AERIAL DISPERSAL OF PARTICLES EMITTED INSIDE PLANT CANOPIES: APPLICATION TO THE SPREAD OF PLANT DISEASES

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Abstract

This work combines numerical, experimental, and theoretical methods to investigate the dispersion of particles inside and above plant canopies. The large-eddy simulation (LES) approach is used to reproduce turbulence statistics and three-dimensional (3-D) particle dispersion within the canopy roughness sublayer (the region of flow significantly modified by the presence of the canopy, extending from ground to about three canopy heights). The Eulerian description of conservation laws of fluid momentum and particle concentration implies that the continuous concentration field is advected by the continuous flow field. Within the canopy, modifications are required for the filtered momentum and concentration equations, because spatial filtering of flow variables and concentration field is inapplicable to a control volume consisting of both fluid and solid elements. In this work, the canopy region is viewed as a space occupied by air only. The sink of airflow momentum induced by forces acting on the surfaces of canopy elements is parameterized as a non-conservative virtual body force that dissipates the kinetic energy of the air. This virtual body force must reflect the characteristic of the surface forces exerted by canopy elements within the control volume, and is parameterized as a “drag force” following standard practice in LES studies. Specifically, the “drag force” is calculated as a product of a drag coefficient, the projected leaf area density, and the square of velocity. Using a constant drag coefficient, this model allows first-order accuracy in reproducing the vertically integrated sink of momentum within the canopy layer for airflows of high Reynolds number. The corresponding LES results of first- and second-order turbulence statistics are in good agreement with experimental data obtained in the field interior, within and just above mature maize canopies. However, the distribution of momentum sink among weak (low velocity) and strong (high velocity) events has not been well reproduced, inferred from the significant underestimation of streamwise and vertical velocity skewness as well as the fractions of vertical momentum flux transported by strong events. Using a velocity-dependent drag coefficient that accounts for the effect of plant reconfiguration (bending of canopy elements due to the aerodynamic drag force),
the “drag force” model leads to LES results of streamwise and vertical velocity skewness as well as the fractions of vertical momentum flux transported by strong events in better agreement with field experimental data. Specifically, modeling the impact of reconfiguration allows strong events to penetrate into deeper canopy regions, reducing the underprediction of streamwise and vertical velocity skewness as well as the vertical momentum flux transported by strong events from 60%, 60%, and 40% to 5%, 20%, and 5%, respectively. On the other hand, the vertically integrated sink of momentum within the canopy layer has been kept approximately the same, so do first- and second-order turbulence statistics.

The link between plant reconfiguration and turbulence dynamics within the canopy roughness sublayer is further investigated. The “reconfiguration drag model” using velocity-dependent drag coefficient is revised to incorporate a theoretical model of the force balance on individual crosswind blades. In the LES, the dimension and degree of the reconfiguration of canopy elements affect the magnitude and position of peak streamwise velocity skewness within the canopy as well as the fractions of vertical momentum flux transported by strong events. The streamwise velocity skewness is shown to be related to the penetration of strong events into the canopy, which is associated with the passage of canopy-scale coherent eddies. With the profile of mean vertical momentum flux constrained by field experimental data, changing the model of drag coefficient induces negligible changes in the vertically integrated “drag force” within the canopy layer. Consequently, first- and second-order turbulence statistics remain approximately the same. However, enhancing the rate of decrease of drag coefficient with increasing velocity increases the streamwise and vertical velocity skewness, the fractions of vertical momentum flux transported by strong events, as well as the ratio between vertical momentum flux transported by relatively strong head-down “sweeps” and relatively weak head-up “ejections”. Note that “sweeps” and “ejections” are defined based on streamwise and vertical velocity fluctuations, and are different from their classical definitions. These results confirmed the inadequacy of describing the effects of canopy-scale coherent structures using just first- and second-order turbulence statistics.

The filtered concentration equation is applied to the dispersion of particles within the canopy roughness sublayer, assuming that a virtual continuous concentration field is advected by a virtual continuous velocity field. A canopy deposition model is used to model the sink of particle concentration associated with the impaction, sedimentation, retention, and re-entrainment of particles on the surfaces of canopy elements. LES results of mean particle concentration field and mean ground deposition rate were evaluated against data obtained during an artificial continuous point-source release experiment. Accounting for the effect of reconfiguration by using a velocity dependent drag coefficient leads to better agreement between LES results and field experimental data of the mean particle concentration field, suggesting the
importance of reproducing the distribution of momentum sink among weak and strong events for reproducing the dispersion of particles. LES results obtained using a velocity-dependent drag coefficient are analyzed to estimate essential properties for the occurrence of plant disease epidemics, i.e., the fraction of particles that escape the canopy (escape fraction) and the growth of the particle plume in the vertical direction. The most interesting finding is that an existing analytical function can be used to model the crosswind-integrated mean concentration field above the canopy normalized by the escape fraction for particles released from the field interior.

Our LES results suggest that the escape fractions of particles released close to the canopy leading edge are greater than those released in the field interior, especially for particles released in the bottom half of the canopy. Effects of the canopy leading edge on the escape fraction can be tracked to the effects on the fractions of particles removed by deposition on modeled “canopy elements” and on the ground. The rate of deposition on canopy elements can be suppressed by enhanced modeled retention and re-entrainment of particles in the region of strong mean wind, while the rate of deposition on the ground can be suppressed by non-negligible mean vertical advection with respect to vertical turbulent transport. Away from the source, the vertical growth of the plume above the canopy-leading-edge area is slower than that above the field interior, due to greater shear of mean streamwise velocity in the internal boundary layer (IBL) than that in the fully-developed canopy roughness sublayer above the canopy.

Spore dispersal downwind from the source field is investigated by representing the infected field as a prescribed constant mean concentration at a reference height near the canopy top. This “source-in-the-mean” model neglects the spatial heterogeneity of infections, release rates, and escape fractions, allowing a first-order accuracy in reproducing the effective source strength of a severely infected field. For dispersion of particles emitted from finite area sources in the atmospheric boundary layer (ABL), pre-existing theoretical models proposed for neutral conditions are extended to unstable conditions. The major effects of buoyancy are accounted for by modifying the profile of vertical velocity variance and considering the ratio between friction and convection velocities. Theoretical predictions of mean concentration profile, plume height, and horizontal transport above the source as well as ground deposition rate downstream from the source are in good agreement with LES results for the plume within the atmospheric surface layer.
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Preface


Chapter 4 is a portion of the manuscript currently under the review as: Pan, Y., E. Follett, M. Chamecki, and H. Nepf (2014) “Strong and weak, unsteady reconfiguration and its impact on turbulent structure within plant canopies,” Phys. Fluids [11]. Permissions from AIP Publishing LLC may be required for future reuse of this work. Fig. 4.1 is a revised version of Fig. 2(b) in Luhar and Nepf (2011) [3], with Copyright 2014 by the Association for the Sciences of Limnology and Oceanography, Inc..

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Chapter 1  |  Introduction

1.1 Motivation

Knowledge of transport processes within and above plant canopies (crops fields, forests, seagrass meadows, etc.) is critical for understanding the spread of biogenic particles (e.g., pollens [13], seeds [14], and spores [15]), the dispersion of pesticide and fungicide spray plumes [16], the emission of volatile organic compounds (e.g., isoprene [17]), the deposition of air pollutants (e.g., ozone [18,19], heavy metals [20], and aerosol particles [21]), the exchange of sensible and latent heat as well as greenhouse gases between vegetation and the atmosphere [22,23], and the trapping of sediments by aquatic plants [24]. The dispersal of biogenic particles is particularly important for understanding plant community dynamics and managing agricultural crops [25]. Seed dispersal influences plant recruitment that affects coexistence and competition in plant communities [14,26], while gene flow from transgenic to non-transgenic crops can occur by wind pollination [27]. Many common plant diseases that destroy important crops are spread by pathogenic fungal spores that disperse through the air [28], causing substantial consequences such as yield reduction [29] and the cost of control [30]. For example, cereal rusts are one of the most important diseases worldwide [31]. The new Ug99 races of the aerially dispersed stem rust pathogen are the most important threat to world wheat production that has emerged in the past 50 years [32,33]. Similarly, the recent aerial incursion into the U.S. of pathogenic spores that cause soybean rust has generated an unprecedented response to this potentially devastating fungal disease [34–36]. The control strategies for plant disease epidemics are typically applied to regional and continental scales of 10
to 1000 kilometers [37]. Nevertheless, the spread of spores on large scales predicted by integrated aerobiological models is highly sensitive to the parameterization of source areas [38], i.e., the dispersal of spores on canopy (horizontal scales corresponding to a few canopy heights) and field scales (a few canopy heights to a few kilometers). For example, early in a plant disease epidemic, most spores are produced and released in the bottom half of the canopy [39]. Given appropriate conditions (e.g., weak UV radiation, high humidity, and moderate temperature fluctuations), the production of spores can be very large, but initially disease spread is slow because the vast majority of the released spores deposit on the ground or canopy elements nearby. Rust diseases observed in the bottom to middle canopy region, for example, usually remain within about one meter horizontally for a long period of time [29]. Once spores escape from the canopy region, they can be transported for very long distances [28,35] due to their small size (1 to 100 µm in diameter) and small settling velocity (0.001 to 0.4 m s$^{-1}$) [40]. In other words, only spores that escape the canopy contribute to the spread of the disease between fields [41], and disease epidemics are usually initiated by the arrival of pathogenic spores from distant locations that are deposited by rain [35]. The product of release rate and escape fraction (fraction of spores that escape the canopy region) has been used as a standard method to quantify emission of spores from agricultural fields [37,42], but field measurements of escape fraction are limited and inaccurate. Most of the current knowledge for escape of spores is based on simple numerical models such as the Lagrangian Stochastic models (LSMs) [4,15,43] and numerical solutions to the mean advection-diffusion equation [43,44]. Results from these studies suggest that the spread of fungal spores depends on the dynamics of turbulence generated by the interaction between vegetation canopy and the atmosphere, and the inadequate representation of vertical turbulent dispersion within the canopy may be responsible for the large discrepancies between model predictions and experimental results [4,43]. In addition, most of the treatments of the near-source plume geometry for long-distance transport models are based on assumptions of instant-mixed grid [38] and Gaussian plumes [37,42], neglecting the role of turbulence characteristics (e.g., shear, heterogeneity, skewness, and coherent structures) in shaping the particle plume. For particles released from point sources located at the canopy top, the three-dimensional (3-D) mean concentration field predicted by Gaussian [45] and quasi-Gaussian [46] plume models are within a
factor of more than 10 of observations, meaning uncertainties are too large to be of practical use in predicting disease spread. A more accurate representation of the geometry of the particle plume on canopy and field scales may also improve the prediction of spore dispersal on large scales.

1.2 Turbulence and Dispersion Inside and Above Plant Canopies

When wind blows over vegetated land, the vegetation canopy first acts as a displaced wall, inducing rough-wall boundary-layer eddies above the displacement height ($\sim 3/4$ canopy height). Within the canopy, wakes are formed behind individual canopy elements. In addition, surface forces acting on the interfaces between airflow and canopy elements dissipate the kinetic energy of the air, appearing as a “drag force” acting on the mean flow within the canopy layer. The presence of “drag force” within the canopy and the absence of “drag force” above the canopy result in an inflected mean velocity profile with an inflection point located near the canopy top, showing a similar shape to that in a free shear layer (mixing layer) formed between two uniform, nearly parallel streams of different velocities [47]. The canopy-shear and the free shear layers are analogous in the instabilities and consequent eddies triggered by the inflected mean wind profile as well as second- and third-order turbulence statistics [47]. The non-linear interactions of rough-wall boundary-layer eddies, canopy-shear-layer vortices, and wake eddies lead to extremely complicated turbulence field within and just above the canopy, a region from ground to approximately three canopy heights, known as the “canopy roughness sublayer” [48,49]. Within this roughness sublayer, turbulence statistics up to the second order have been successfully reproduced by second-order closure models using the canopy-mixing layer analogy [4,50], where the local mixing length scale (mean velocity at the canopy top divided by mean shear at the canopy top) is used to parameterize turbulent transport [47]. However, third-order closure models failed to reproduce third-order turbulence statistics (streamwise and vertical velocity fluctuations) [51]. Large-eddy simulation (LES) models assume that the canopy region consisting of both airflow and canopy elements is occupied by air only, and the surface forces acting on the interfaces between airflow and canopy elements
are parameterized as a virtual body force acting on the volume of the virtual fluid [52–57]. This virtual body force must inherit the characteristics of the actual surface forces, which depend on the surface area of canopy elements and the velocity of the airflow. Statistically it appears as a “drag force” calculated as a product of a drag coefficient, the leaf area density, and the squared of filtered velocity of the virtual fluid. A constant drag coefficient was used by earlier LES studies to model the effects of canopy elements on the airflow for high Reynolds number conditions [52–57]. These LES studies successfully reproduced first- and second-order turbulence statistics, but significantly underestimated (≳ 50%) streamwise and vertical velocity skewness as well as the vertical momentum flux transported by strong events (high velocity) [53–57].

The transport of tracers (e.g., scalars and particles) within the canopy roughness sublayer is also a difficult problem, because in many cases the transport of tracers within the canopy consists of critical contribution from near-field dispersion [58,59]. Here near-field indicates that the time since the release of tracer is short compared with the Lagrangian time scale (a measure of the coherence or persistence of turbulent motions), and therefore the dispersion depends on the velocity histories of the tracer particles [60,61]. This is not a diffusive process, and cannot be described by a diffusion equation. In contrast, dispersion in the far-field (the time since the release of tracer is long compared with the Lagrangian time scale) no longer depends on the histories of the tracer particles, which becomes a diffusive process that can be described by a diffusion equation [60,61]. The solution to the advection-diffusion equation must be modified to account for the contribution from near-field non-diffusive dispersion in order to provide realistic estimation of the mean concentration field for tracers released inside plant canopies [62]. Assuming locally homogeneous turbulence about each source location for near-field dispersion, theoretical solutions of two-dimensional mean concentration field show good agreement with LSM predictions [62]. The use of LSMs has been the preferred approach to study dispersion of scalars [63–65] and particles [4,37,66,67] within the canopy roughness sublayer. Nevertheless, a comprehensive comparison between LSM predictions and experimental data of 3-D particle dispersion shows that model predictions are sensitive to the parameterization of the Lagrangian time scale, while the existing highly empirical parameterization schemes of the Lagrangian time scale do not reproduce vertical dispersion accurately [4].
Lagrangian time scale not only measures the coherence and persistence of turbulent motions governing near-field dispersion, but also determines the eddy-diffusivity for far-field dispersion [60]. The issue associated with the Lagrangian time scale can be avoided by explicit representation of turbulence within the canopy roughness sublayer, e.g., the LES approach, in which the concentration field is assumed to occupy the entire canopy region consisting of both the airflow and canopy elements, and the virtual continuous concentration field is assumed to be transported by the virtual continuous velocity field [68]. Compared with results given by an LSM using turbulence statistics and time scales predicted by the LES model, the LES results show a higher mean plume height (centroid of the plume), suggesting an enhanced vertical dispersion [68]. However, comprehensive comparison between LES results and experimental data of 3-D particle dispersion is still lacking.

Turbulence and dispersion within and above infinite, horizontally homogeneous canopy (representing the field interior) have not been well reproduced, while the reality is even more complicated. The land surface is a patchwork of vegetation and land use, while airflow characteristics [7,8,69,70] and particle dispersion patterns [71] at canopy edges are different from those in the field interior (where turbulence has adjusted to the canopy drag). Measurements suggest that pathogenic fungal spores released at the canopy leading edge tend to disperse farther than those released in the field interior [71]. Canopy leading edge flows have been studied using laboratory [72,73] and field [74–76] experiments, theoretical models [8], and LES models [7,56,69,70,77]. The effects of canopy leading edge on the dispersion of particles have important implications on landscape arrangement (e.g., modifying the field arrangement for agricultural crops to reduce the risk of disease epidemics), but quantitative estimates of these effects are unavailable.

Above the canopy roughness sublayer, both numerical and theoretical approaches are better developed compared with those within the roughness sublayer. The LES approach is able to reproduce velocity and temperature statistics accurately for airflows over homogeneous underlying surfaces and across roughness changes, for both neutral and unstable conditions [78,79]. LES results of particle dispersion for neutral conditions agree well with measurements from point- and area-source release experiments [80,81]. The Monin-Obukhov similarity theory describes the turbulence statistics observed within the atmospheric surface layer (the bottom 10% to 20% of the atmospheric boundary layer (ABL)) for weakly stable to moderately
unstable conditions [82]. The gradient-diffusion approach holds in the atmospheric surface layer as well [83]. Therefore theoretical solutions to the advection-diffusion equation have been obtained for particles emitted from horizontally homogeneous sources [84–86], point or line sources [10, 87–90], and finite area sources [91–93]. The dispersion of particles from finite area sources represents a difficult problem for theoretical solutions due to spatial heterogeneity and local advection, but is of practical interest due to commonly existing patchwork of vegetation and land use. Chamecki and Meneveau (2011) proposed a theoretical model for this problem for neutral conditions, which may become more practically useful if it can be extended to unstable conditions. The amount and distance of particle transport in the unstable ABL are greater than those in the neutral and stable ABL, as suggested by both field measurements and numerical simulations [94], enhancing the potential to initiate plant disease epidemics.

1.3 Open Research Questions

Reliable estimation of the escape fraction requires accurate reproduction of 3-D field experimental data of particle dispersion, which is beyond the capability of simple numerical models that do not resolve canopy-scale turbulent eddies. LES is the best approach to simulate the complex turbulence dynamics within the canopy roughness sublayer, but a known weakness of earlier LES studies is the underestimation of streamwise and vertical velocity skewness as well as the fractions of vertical momentum flux transported by strong events (high velocity) within plant canopies [53–57]. This weakness may lead to uncertainties in predictions of particle dispersion due to the importance of strong events [43], but has not been solved through more than 20 years of efforts since the pioneering LES study of Shaw and Schumann (1992) [52]. Increasing grid resolution [55, 95], considering the geometric structure of individual plants [95], and representing plant motion as a linear mode of vibration [96] have not eliminated the underprediction of velocity skewness and the vertical momentum transported by strong events. Accounting for the effects of temperature stratification is unlikely to reduce the underestimation of skewness, because largest skewness values were observed under neutral conditions [97]. Is the LES approach capable of reproducing experimental data of skewness and the stress fractions carried by strong events? Are any important physical mechanisms missing
in the LES, preventing the models from reproducing experimental data? Given the velocity skewness and strong events well reproduced, is the LES approach capable of accurately reproducing 3-D dispersion of particles?

The Lagrangian time scale, a critical parameter used in theoretical solutions [62] and LSMs [4], is directly related to canopy-shear-layer coherent structures. These coherent structures behave similarly to the Kelvin-Helmholtz (KH) coherent structures generated in the free shear layer, and therefore are also called “KH coherent structures” by earlier studies of the canopy-shear layer [24, 48, 98]. These shear-layer eddies dominate the transport of momentum inside plant canopies [99], and are related to the streamwise and vertical velocity skewness [100]. Scalar flux at the canopy top has also been linked to strong events associated with canopy-shear-layer eddies [101, 102]. However, LSMs applied to the canopy roughness sublayer either assume Gaussian velocity distribution [4, 37, 63–67], or the incorporation of non-Gaussian velocity statistics has not improved predictions of mean concentration profiles [63, 103]. The inclusion of the skewness of vertical velocity, in particular, induces negligible changes in LSM predictions of mean concentration profiles [62]. Do LES results suggest connections between skewness and canopy-shear-layer coherent structures? How does the underestimation of velocity skewness and the vertical momentum flux transported by strong events affect results of particle dispersion?

The fractions of particles that escape the canopy region (i.e., escape fraction) links the dispersion of spores on canopy scales to the spread of spores on field scales [41] as well as the occurrence of plant disease epidemics on regional and continental scales [28, 35]. How does the escape fraction depend on the location of the source (height inside the canopy and the distance from the canopy edge)? What are the controlling factors of the escape fraction (e.g., properties of the flow field, the particle, and the canopy)?

Dispersion of particles within the canopy is driven by complex turbulent flow, and is further complicated by deposition of particles on canopy elements. Is it possible to reproduce the mean concentration field above the canopy without intensive numerical simulation of dispersion inside the canopy? How does the mean particle concentration above the canopy relate to the escape fraction (e.g., proportionality, dependence on source location)? What are the factors determining the shape of the particle plume above the canopy? Is it possible to find a theoretical
model to provide realistic estimation of particle dispersion above the canopy and within the canopy roughness sublayer?

A practical field-scale problem is the dispersion of particles emitted from finite area sources, for which LES results and analytical solutions have been obtained for neutral conditions with the assumption that the source field can be represented as a constant mean concentration field [92]. How good is this assumption? What discrepancies from the reality can be caused by using this assumption? Extending the theoretical solutions from neutral to unstable conditions is of practical interest, particularly for the spread of plant diseases. Can the theoretical models for neutral conditions be extended to unstable conditions? What are the major effects of the unstable atmospheric temperature stratification?

These open research questions will be addressed in Chapters 3–6, with detailed procedures introduced in Section 1.4. The methodology for numerical simulation and model evaluation is described in Chapter 2, with relevant features re-introduced in Chapters 3–6. Conclusions are given in Chapter 7, with suggestions for future research. Although these questions are raised by the dispersion of pathogenic fungal spores and the application to plant disease epidemics, they are relevant to a wide range of problems associated with vegetation canopy flows. The dispersion of other biogenic particles, such as small seeds and pollens, behave similarly to that of fungal spores, except for experiencing a larger settling velocity. An LES model that successfully reproduces turbulence statistics and particle dispersion within the canopy roughness sublayer is also useful for understanding the transport of other species (e.g., sensible and latent heat, greenhouse gases, air pollutants, and river sediments) associated with various terrestrial and aquatic canopies.

1.4 Procedures to Approach Research Questions

This work combines numerical, experimental, and theoretical methods to investigate the dispersion of particles on canopy (Chapters 3–5) and field (Chapter 6) scales. The parameterization schemes of vegetation canopy in LES models are introduced in Section 2.1. The details of the LES model are described in Section 2.2, including the governing equations, subgrid-scale (SGS) model, discretization, and boundary conditions. Experimental data from Gleicher et al. (2014) [4] and Wilson et al. (1982) [1] (described in Section 2.3) were used to evaluate LES results of turbulence
statistics, mean particle concentration field, and mean ground deposition rate. The model evaluation strategies are also explained in Section 2.3.

The starting point of this work is to investigate the capability of LES approach to reproduce field experimental data of turbulence and particle dispersion within the canopy roughness sublayer in the field interior (represented as infinite, horizontally uniform canopy) under neutral conditions, which is the most simplified problem on the canopy scale (Chapter 3). The canopy layer is viewed as a continuum of fluid, and the surface forces acting on the interfaces between the airflow and canopy elements are parameterized as a virtual body force acting on the volume of the virtual fluid, following the pioneer LES study of Shaw and Schumman (1992) [52]. This virtual body force appears as a “drag force”, dissipating the kinetic energy of the virtual fluid. LES runs have been conducted using two formulae of drag coefficient for the model of “drag force”: (1) a constant drag coefficient used in earlier LES studies [52–57], and (2) a velocity-dependent drag coefficient accounting for the effects of reconfiguration (bending of canopy elements induced by the aerodynamic drag force). LES results are evaluated against field experimental data of turbulence statistics up to the third order and 3-D mean particle concentration field. LES using a velocity-dependent drag coefficient yields better reproduction of the mean concentration field (Section 3.3), providing results for reliable estimation of the escape fraction for particles of various settling velocities released at various heights (Section 3.4.1). Theoretical models describing the crosswind-integrated mean concentration field above the canopy are investigated in Section 3.4.2.

The effect of reconfiguration has been shown to be critical for accurate reproduction of strong events and mean particle concentrations (shown in Chapter 3), and therefore is further investigated in Chapter 4. LES results show that the dimension and degree of reconfiguration modify the magnitude and vertical position of peak skewness and changes the stress fractions carried by strong events. These results also suggest the link between skewness and canopy-scale coherent structures.

The effects of canopy leading edge on the dispersion of particles are investigated in Chapter 5. Quantitative estimation of the escape fraction and analysis of the crosswind-integrated mean concentration field above the source are obtained from LES for particles released from various locations (height inside the canopy and distance downstream from the canopy leading edge). The link between dispersion on the canopy scale and that on the field scale is discussed, in particular, for the
treatment of the source field in Chapter 6.

A pre-existing theoretical model for dispersion of particles emitted from finite area sources in the neutral atmospheric surface layer [92] are extended to include the effect of unstable atmospheric temperature stratification in Chapter 6. Theoretical predictions for the mean concentration profile, plume height, and horizontal transport above the source, as well as ground deposition flux downwind from the source are compared with LES results (Section 6.3). The theoretical model is also compared with earlier theoretical solutions for simplified problems (e.g., the ground deposition rate downstream from a crosswind line source [10, 87]; Section 6.4).
Chapter 2  Methodology

2.1 Effects of Canopy on Airflow and Dispersion

2.1.1 Effects of Canopy on Airflow

The Eulerian form of Boussinesq approximation of Navier-Stokes equation in a rotating frame of reference describes the motion of air in the atmospheric boundary layer (ABL). The continuity equation is,

$$\nabla \cdot \mathbf{u} = 0,$$

(2.1)

where $\mathbf{u}$ is the velocity of the fluid. The momentum equation is written as,

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u} \mathbf{u}) = -\frac{1}{\rho_0} \nabla p + \frac{\rho}{\rho_0} \mathbf{g} + \nu \nabla^2 \mathbf{u} - 2 \Omega \times \mathbf{u},$$

(2.2)

where $\nu$ is the kinematic viscosity of air, $\mathbf{g}$ is the effective gravitational acceleration on Earth, and $\Omega$ is the angular velocity of Earth with respect to its own axis. Variables $p$ and $\rho$ are the perturbations of pressure and density of the fluid with respect to their base state $p_0$ and $\rho_0$, respectively. For low Mach number flow (i.e., $|\mathbf{u}| \ll c$, where $c$ is the speed of sound), the ideal gas law leads to $\rho/\rho_0 \approx -\theta/\theta_0$, where $\theta$ is the perturbation of potential temperature with respect to its base state $\theta_0$. The conservation of internal energy is written as,

$$\frac{\partial \theta}{\partial t} + \nabla \cdot (\mathbf{u} \theta) = \alpha_\theta \nabla^2 \theta,$$

(2.3)
where $\alpha_\theta$ is the thermal diffusivity. Eqs. (2.1)–(2.3) form a closed system of equations, and can be solved with proper initial and boundary conditions. However, environmental flows are associated with large Reynolds numbers ($Re \sim 10^7$), which exceeds the currently available computational power. A spatial filtering procedure is necessary for simulation of environmental flows, known as the large-eddy simulation (LES) approach. Even if the computational power were enough to resolve all turbulent scale associated with $Re \sim 10^7$, the direct numerical simulation (DNS) is inapplicable to environmental flows near the Earth’s surface, due to non-trivial boundary conditions formed by irregular and complex arrangement of roughness elements (e.g., trees, crops, grasses, buildings, etc.). Models that do not resolve individual roughness elements also require a spatial filtering procedure, such as the large-eddy simulation (LES) approach.

Filtering Eqs. (2.1)–(2.3) yields,

$$\nabla \cdot \tilde{u} = 0, \quad (2.4)$$

$$\frac{\partial \tilde{u}}{\partial t} + \nabla \cdot (\tilde{u} \tilde{u}) = -\frac{1}{\rho_0} \nabla \tilde{p} - \frac{\tilde{\theta}}{\theta_0} g + \nu \nabla^2 \tilde{u} - 2\Omega \times \tilde{u}, \quad (2.5)$$

$$\frac{\partial \tilde{\theta}}{\partial t} + \nabla \cdot (\tilde{u} \tilde{\theta}) = \alpha_\theta \nabla^2 \tilde{\theta}. \quad (2.6)$$

If the filtering and differential operators are commutative, then we obtain the predictive equations for filtered properties,

$$\nabla \cdot \tilde{u} = 0, \quad (2.7)$$

$$\frac{\partial \tilde{u}}{\partial t} = -\nabla \cdot (\tilde{u} \tilde{u}) - \frac{1}{\rho_0} \nabla \tilde{p} - \frac{\tilde{\theta}}{\theta_0} g + \nu \nabla^2 \tilde{u} - 2\Omega \times \tilde{u} - \nabla \cdot (\tilde{\omega} \tilde{u} - \tilde{u} \tilde{\omega}), \quad (2.8)$$

$$\frac{\partial \tilde{\theta}}{\partial t} = -\nabla \cdot (\tilde{u} \tilde{\theta}) + \alpha_\theta \nabla^2 \tilde{\theta} - \nabla \cdot (\tilde{\omega} \tilde{\theta} - \tilde{u} \tilde{\omega}). \quad (2.9)$$

Note that the commutation of filtering and differential operators in Eqs. (2.1)–(2.3) is only guaranteed for $u$, $p$, and $\theta$ that are continuous in time to the first-order derivatives and in space to the second-order derivatives and for spatially homogeneous and isotropic filtering. Here Eqs. (2.7)–(2.9) form a closed system of equations if terms $\nabla \cdot (\tilde{u} \tilde{u} - \tilde{u} \tilde{u}) = \nabla \cdot \sigma$ and $\nabla \cdot (\tilde{u} \tilde{\theta} - \tilde{u} \tilde{\theta}) = \nabla \cdot q$ can be modeled using resolved flow variables ($\tilde{u}$, $\tilde{p}$, and $\tilde{\theta}$). In LES, $\sigma$ and $q$ are known as
subgrid-scale (SGS) momentum and heat fluxes, respectively.

The canopy region is occupied by both the airflow and canopy elements, and flow variables (e.g., $u$, $p$, and $\theta$) are undefined within the volume occupied by solid elements. Mathematically the spatial filtering procedure is not applicable to the canopy region. Physically the solid elements affect the velocity field through surface forces, acting as a sink of momentum. The canopy elements may also exchange heat with the airflow, acting as a source or sink of heat. The exchange of heat between canopy elements and the airflow is beyond the scope of this work, and here we assume no perturbation of the filtered potential temperature field with respect to the base state (i.e., $\tilde{\theta} = 0$). This assumption is a good approximation if the domain of interest is confined to the region within and just above short and dense vegetation canopies (e.g., mature maize canopy) at mid-latitudes during daytime on non-precipitating, windy days in summer and fall (e.g., observed by Wilson et al. (1982) [1] and Gleicher et al. (2014) [4]). However, this assumption becomes a poor assumption if the domain of interest consists of the entire atmospheric boundary layer (ABL), or within tall canopies (e.g., forests) where strong temperature stratifications have been observed (e.g., Dupont and Patton (2012) [97]). With the assumption of $\tilde{\theta} = 0$, we employ the LES approach by viewing the canopy layer as a continuum fluid. An extra term, $d$, is added to Eq. 2.8, parameterizing the momentum sink caused by the surfaces of canopy elements. Eq. (2.8) is rewritten as,

$$
\frac{\partial \tilde{u}}{\partial t} = -\nabla \cdot (\tilde{u} \tilde{u}) - \frac{1}{\rho_0} \nabla \tilde{p} + \nu \nabla^2 \tilde{u} - 2\Omega \times \tilde{u} - \nabla \cdot \sigma + d,
$$

(2.10)

where the additional force term ($d$) appears as a body force acting on the volume of the virtual fluid. This virtual body force is non-conservative, dissipating the kinetic energy of the virtual fluid. Eqs. (2.7) and (2.10) form a closed system of equations if $d$ can be modeled using resolved flow variables ($\tilde{u}$ and $\tilde{p}$).

The virtual body force ($d$) must inherit characteristics of surface forces acting on the interfaces between canopy elements and the air, so it must depend on the distribution of surface area of canopy elements and the velocity field. Shaw and Schumann (1992) [52] proposed the parameterization,

$$
d = -C_d a |\tilde{u}| \tilde{u},
$$

(2.11)
where the drag coefficient $(C_d)$ and the leaf-area density $(a)$ characterize the surfaces of canopy elements, and $\tilde{u}$ characterizes the velocity field. This model implies that the cluster of canopy elements exerts a total force $(d)$ that is aligned with the filtered velocity $(\tilde{u})$, which requires at least the assumption that the canopy is isotropic. Considering that the canopy is anisotropic, so that the effective leaf area density can be different for streamwise, spanwise, and vertical velocity components, we introduced a second-order projection tensor $(P)$ for leaf area density $(a)$. Then Eq. (2.11) is re-written as

$$d = -C_d (aP) \cdot (|\tilde{u}| \tilde{u}). \tag{2.12}$$

In this work, we assume that $P$ only consists of non-zero diagonal components (i.e., $P = P_x e_x e_x + P_y e_y e_y + P_z e_z e_z$), so that $d$ only dissipates kinetic energy ($\tilde{u} \cdot d \leq 0$). In reality, surfaces of canopy elements can re-direct the flow, and therefore re-distribute the components of kinetic energy as well. These effects may lead to non-zero off-diagonal components for the projection tensor $(P)$. Values of the diagonal components $(P_x, P_y,$ and $P_z)$ are allowed to be different, representing the anisotropy of the canopy. We assume that individual surfaces of canopy elements facing either streamwise, spanwise, or vertical directions, so that $P_x + P_y + P_z = 1$. In reality, surfaces of canopy elements can face any directions, so that the model $P_x + P_y + P_z = 1$ may not hold. In addition, we assume that the projected leaf area density $(aP)$ is static, and effects of the deformation of canopy surfaces (such as bending due to aerodynamic drag) are lumped into the drag coefficient, $C_d$. The spatial distribution of canopy surfaces is assumed horizontally homogeneous, so that the leaf area density $(a)$ only depends on height. The projection coefficients $(P_x, P_y,$ and $P_z)$ are assumed constant within the entire canopy. In reality, the spatial distribution of canopy surfaces can be horizontally heterogeneous, and therefore $a$, $P_x$, $P_y$, and $P_z$ are functions of space.

The drag coefficient accounts for the effects of the flow field and the deformation of canopy surfaces. In reality, the flow field is anisotropic, because the streamwise velocity component is usually much larger than the spanwise and vertical components. The horizontal surfaces are usually flat (e.g., leaves), while the vertical surfaces are usually cylinders (e.g., stems). Therefore, the drag coefficient is at least a second-order tensor consisting of non-zero diagonal components of different values.
These components must depend on the Reynolds number, \( Re = ULv/\nu \), which measures the relative importance of inertia and viscous forces of the flow. Here \( U \) is the characteristic velocity scale for motions in the direction of interest, and \( L_v \) is the characteristic length scale of canopy elements, such as the width of leaves and the diameter of stems. In addition, the deformation of canopy surfaces can be represented by a second-order tensor consisting of both non-zero diagonal and off-diagonal components. These components must depend on the Cauchy number, \( Ca \), which measures the relative importance of the inertia forces of the flow and the bending rigidity of canopy elements (see the definition of Cauchy number (\( Ca \)) for a flexible blade in cross flow in Chapter 4). In this work, a scalar drag coefficient (\( C_d \)) is modeled as either a constant or a function of the Cauchy number (\( Ca \)). Both models assume no dependence of drag coefficient on the Reynolds number (\( Re \)). The model \( C_d = \text{constant} \) assumes no deformation of canopy surfaces, while the model \( C_d = C_d(Ca) \) assumes that deformation appears as a rate of expansion/contraction that is equal in streamwise, spanwise, and vertical directions (the same diagonal components and zero off-diagonal components).

### 2.1.2 Effects of Canopy on Dispersion

The dispersion of monodisperse particles is modeled as a continuous concentration field (\( C \)). The Eulerian form of the conservation of particle concentration is written as,

\[
\frac{\partial C}{\partial t} + \mathbf{v}_p \cdot \nabla C = D \nabla^2 C + Q,
\]

where \( Q \) is the source/sink term, \( \mathbf{v}_p \) and \( D \) are the velocity and diffusivity of particles. Note that we assume particles do not affect the flow field. In the asymptotic regime of small particle inertia, \( \mathbf{v}_p \approx \mathbf{u} + \tau_p \mathbf{a}_p \), where \( \tau_p \) and \( \mathbf{a}_p \) are the relaxation time and acceleration of the particle [104]. In the asymptotic regime of dense particle, \( \mathbf{a} = \mathbf{g} + \mathbf{a}_f \), where \( \mathbf{a}_f \) is the acceleration of the fluid. For \( \mathbf{a}_f \ll \mathbf{g} \), we obtain \( \mathbf{v}_p \approx \mathbf{u} + \tau_p \mathbf{g} = \mathbf{u} - w_s \mathbf{e}_z \), where \( w_s \) is the gravitational settling velocity. Using these assumptions, we write the filtered concentration equation as,

\[
\frac{\partial \tilde{C}}{\partial t} + \nabla \cdot (\mathbf{u} \tilde{C}) - w_s \mathbf{e}_z \cdot \nabla \tilde{C} = D \nabla^2 \tilde{C} + \tilde{Q},
\] (2.14)
If the filtering and differential operators are commutative, then we obtain the predictive equation for filtered concentration,

$$\frac{\partial \tilde{C}}{\partial t} = -\nabla \cdot (\tilde{u} \tilde{C}) - w_s e_z \cdot \nabla \tilde{C} + D \nabla^2 \tilde{C} + \tilde{Q} - \nabla \cdot (\tilde{u} C - \tilde{u} \tilde{C}) \quad (2.15)$$

Similar to Eqs. (2.1)–(2.3), the commutation of filtering and differential operators is only guaranteed for concentration field \((C)\) continuous in time to the first-order derivatives and in space to the second-order derivatives and for spatially homogeneous and isotropic filtering. With the closed system formed by Eqs. (2.7)–(2.9), Eq. (2.15) is closed if the term \(\nabla \cdot (\tilde{u} C - \tilde{u} \tilde{C}) = \nabla \cdot \pi^C\) can be modeled using filtered variables \((\tilde{u} \text{ and } \tilde{C})\). In LES, \(\pi^C\) is known as the SGS concentration flux, .

Within the canopy, the concentration field \((C)\) is undefined within the volume occupied by solid elements, nor is the concentration filed advected by a continuous velocity field occupying the entire canopy region. Mathematically, the spatial filtering procedure is inapplicable to Eq. (3.3) within the canopy. Physically, particles moving through spaces between canopy elements impact on, stick to, and rebound from the surfaces of solid elements, appearing as a sink of the concentration. The standard continuum equation for concentration is applied to the dispersion of particles by adding a term \((S_p)\) to Eq. 2.15 to mimic the sink of concentration associated with the deposition of particles on surfaces of canopy elements. Eq. (2.15) is rewritten as,

$$\frac{\partial \tilde{C}}{\partial t} = -\nabla \cdot (\tilde{u} \tilde{C}) + D \nabla^2 \tilde{C} + \tilde{Q} - \nabla \cdot \pi^C + S_p \quad (2.16)$$

With the closed system formed by Eqs. (2.7) and (2.10), Eq. (2.16) is closed if \(S_p\) can be modeled using filtered variables \((\tilde{u} \text{ and } \tilde{C})\). In this work, \(S_p\) is parameterized using a revised version of the model introduced by Aylor and Flesch (2001) [67], which employs many empirical assumptions and parameters to model sedimentation, impaction, as well as retention and re-entrainment of particles on canopy elements (described in detail in Appendix A). Lagrangian stochastic models (LSMs) using this canopy deposition model yield results of mean concentration field in good agreement with measurements obtained for Lycopodium spores released from the upper half of the maize canopy [4,67]. In this work, this model was implemented
into the LES model without manipulating the empirical parameters, whereas these parameters may change due to different treatments of flow dynamics in LSMs and LES models. This model may be inaccurate to estimate the deposition of particles released from the bottom half of the canopy or the deposition of other types of particles (e.g., pollens) on other types of canopies (e.g., vineyards).

### 2.2 Large-Eddy Simulation Model

In this work, two sets of simulations were designed for different domains of interest. The first domain is confined to the region within and just above mature maize canopies (i.e., the canopy roughness sublayer; Chapters 3–5), while the second domain consists the entire ABL above the vegetation canopy (Chapter 6). As a result, these two sets of simulations use different governing equations and boundary conditions.

#### 2.2.1 Governing Equations and SGS Model

In Chapters 3–5, the model resolves the canopy layer, solving the closed system of equations formed by Eqs. (2.7), (2.10), and (2.16). In Chapter 6, the model does not resolve the canopy layer, solving the closed system of equations formed by Eqs. (2.7)–(2.9) and (2.15). For kinetic energy and mass conservation, the momentum equations (Eqs. (2.8) and (2.10)) are written in the rotational form. Viscous and diffusion terms ($\nu \nabla^2 \tilde{u}$, $\alpha_\theta \nabla^2 \tilde{\theta}$, and $D \nabla^2 \tilde{C}$) are neglected because these terms are orders of magnitude smaller than the advection terms [81,105]. In this work, we also neglected the Coriolis term ($2\Omega \times \tilde{u}$). In Chapters 3–5, the flow is driven by a mean pressure gradient force, as in channel flow, so that an extra term ($\left(1/\rho_0\right)\nabla p$) is added to Eq. (2.10). The governing equations are written as,

\[
\nabla \cdot \tilde{u} = 0, \quad (2.17)
\]

\[
\frac{\partial \tilde{u}}{\partial t} = -\tilde{\omega} \times \tilde{u} - \frac{1}{\rho_0} \nabla \tilde{p}^* - \nabla \cdot \tilde{\tau} + \frac{1}{\rho_0} \nabla \tilde{p}, \quad (2.18)
\]

\[
\frac{\partial \tilde{C}}{\partial t} = -\nabla \cdot (\tilde{u} \tilde{C}) - \nabla \cdot \tilde{\pi}^C + S_p. \quad (2.19)
\]
Here $\tilde{\omega} = \nabla \times \tilde{u}$ is the filtered vorticity, $\tilde{p}^\ast = \tilde{p} + \rho_0 \tilde{u} \cdot \tilde{u}/2 + \rho_0 \text{tr}(\sigma)/3$ is the modified pressure, and $\tau$ is the deviatoric part of the SGS stress tensor ($\sigma$).

In Chapter 6, the flow is driven by a constant mean wind at the top of the domain. The effects of unrealistic boundary conditions associated with the differences between the modeled flow field and the real ABL with the presence of Coriolis force are discussed in Section 2.2.3. The governing equations are written as,

$$\nabla \cdot \tilde{u} = 0,$$

$$\frac{\partial \tilde{u}}{\partial t} = -\tilde{\omega} \times \tilde{u} - \frac{1}{\rho_0} \nabla \tilde{p}^\ast - \tilde{\theta} \frac{\nabla \tilde{\theta}}{\theta_0} g - \nabla \cdot \tau,$$

$$\frac{\partial \tilde{\theta}}{\partial t} = -\nabla \cdot (\tilde{u} \tilde{\theta}) - \nabla \cdot \mathbf{q},$$

$$\frac{\partial \tilde{C}}{\partial t} = -\nabla \cdot (\tilde{u} \tilde{C}) - \nabla \cdot \mathbf{\pi}^C.$$

In both approaches, the SGS momentum flux is modeled using the Smagorinsky model based on concepts of eddy-diffusivity and mixing length,

$$\tau = \tilde{u} \tilde{u} - \hat{\tau} \hat{u} = -2(c_{s,\Delta})^2 |\hat{S}|\hat{S},$$

where $\Delta$ is the grid spacing and $c_{s,\Delta}$ is the corresponding Smagorinsky coefficient, while $\hat{S} = [\nabla \hat{u} + (\nabla \hat{u})^T]/2$ is the resolved strain rate tensor (with superscript “T” indicating the transverse of a second-order tensor). On a test grid spacing of $\alpha \Delta$, the SGS momentum flux is modeled as,

$$T = \tilde{u} \tilde{u} - \hat{\tau} \hat{u} = -2(c_{s,\alpha\Delta})^2 |\hat{S}|\hat{S},$$

where $c_{s,\alpha\Delta}$ is the corresponding Smagorinsky coefficient, and $\hat{S} = [\nabla \hat{u} + (\nabla \hat{u})^T]/2$ is the resolved strain rate tensor on the test grid. The difference between $T$ and $\hat{\tau}$ is written as,

$$L = T - \hat{\tau} = (\tilde{u} \tilde{u} - \hat{\tilde{u}} \hat{u}) - (\hat{\tilde{u}} \hat{\tilde{u}} - \hat{u} \hat{u}).$$

We assume that the term $\tilde{u} \tilde{u} - \hat{\tilde{u}} \hat{u}$ vanishes, and therefore $L$ can be estimated using resolved velocity fields $\tilde{u}$ and $\hat{\tilde{u}}$. This assumption holds for spectral-cut filtering, but may not hold for other types of filtering, such as the local spatial-average filtering. Using Eqs. (2.24) and (2.25), we model the difference between $T$ and $\hat{\tau}$.
as,

$$M = -2(c_s \Delta)^2 \left( \frac{\alpha^2}{c_s^2} \alpha^2 |\hat{S}| \hat{S} - |\tilde{S}| \tilde{S} \right), \quad (2.27)$$

where the parameter $\beta = \frac{c_s^2}{c_s \Delta} \alpha$ can be determined by minimizing the difference between $L$ and $M$. The minimizing procedure was conducted for averaging along the pathlines of fluid particles by Bou-Zeid et al. (2005), providing the scale-dependent Lagrangian dynamic Smagorinsky SGS model [78].

The SGS heat flux is modeled using the eddy-diffusivity approach,

$$q = \tilde{u} \theta - \tilde{u} \hat{\theta} = -\frac{1}{Pr_{SGS}} (c_s \Delta)^2 |\tilde{S}| \nabla \hat{\theta}, \quad (2.28)$$

where the SGS Prandtl number $Pr_{SGS} = 0.4$ [79]. We neglect the dependence of the SGS Prandtl number on the atmospheric temperature stratification.

The SGS concentration flux is modeled using the eddy-diffusivity approach,

$$\pi^C = \tilde{u} C - \tilde{u} \tilde{C} = -\frac{1}{Sc_{SGS}} (c_s \Delta)^2 |\tilde{S}| \nabla \tilde{C}, \quad (2.29)$$

where the SGS Schmidt number $Sc_{SGS} = 0.4$ [81].

### 2.2.2 Discretization Approaches

The systems of Eqs. (2.17)-(2.19) and Eqs. (2.20)-(2.23) can be solved using similar numerical approaches (described in detail by Albertson and Parlange (1999) [106]). The model employs a fully explicity second-order Adams-Bashforth scheme, so that

$$\tilde{u}^t + \Delta t = \tilde{u}^t + \Delta t \left( \frac{3}{2} \text{RHS}_u^t - \frac{1}{2} \text{RHS}_u^{t-\Delta t} \right), \quad (2.30)$$

where RHS$_u$ denotes the right-hand-side (RHS) of the momentum equations (Eqs. (2.18) and (2.21)). Time advance for potential temperature ($\hat{\theta}$) and particle concentration ($\tilde{C}$) are conducted similarly. The momentum and internal energy equations are discretized using pseudo spectral approach in horizontal directions and second-order centered finite-difference approach in the vertical direction. A staggered grid is used in the vertical direction, having the vertical component of velocity ($\tilde{w}$) at heights $n \Delta z$, and the other variables at heights $[n + (1/2)] \Delta z$, where
\(n\) is an integer number \((0 \leq n \leq N_z)\). The velocity field is discretized as

\[
\tilde{u}'(x, y, z) = \sum_{k_x} \sum_{k_y} \tilde{u}'(k_x, k_y, z)e^{i(k_x x + k_y y)},
\]

where \(\tilde{u}\) is the complex Fourier amplitudes associated with the variable \(\tilde{u}\), \(k_x\) and \(k_y\) are the wavenumbers in the \(x\) and \(y\) directions with summations over integer wavenumbers \(-N_x/2 + 1 \leq k_x \leq N_x/2\) and \(-N_y/2 + 1 \leq k_y \leq N_y/2\), and \(i = \sqrt{-1}\).

The first-order spatial derivatives are calculated as,

\[
\frac{\partial}{\partial x} \tilde{u}'(x, y, z) = \sum_{k_x} \sum_{k_y} \tilde{u}'(k_x, k_y, z)(ik_x)e^{i(k_x x + k_y y)},
\]

\[
\frac{\partial}{\partial y} \tilde{u}'(x, y, z) = \sum_{k_x} \sum_{k_y} \tilde{u}'(k_x, k_y, z)(ik_y)e^{i(k_x x + k_y y)},
\]

\[
\frac{\partial}{\partial z} \tilde{u}'(x, y, z - (\Delta z/2)) = \frac{\tilde{u}'(x, y, z) - \tilde{u}'(x, y, z - \Delta z)}{\Delta z}.
\]

The second-order spatial derivatives are calculated as,

\[
\frac{\partial^2}{\partial x^2} \tilde{u}'(x, y, z) = \sum_{k_x} \sum_{k_y} \tilde{u}'(k_x, k_y, z)(-k_x^2)e^{i(k_x x + k_y y)},
\]

\[
\frac{\partial^2}{\partial y^2} \tilde{u}'(x, y, z) = \sum_{k_x} \sum_{k_y} \tilde{u}'(k_x, k_y, z)(-k_y^2)e^{i(k_x x + k_y y)},
\]

\[
\frac{\partial^2}{\partial z^2} \tilde{u}'(x, y, z) = \frac{\tilde{u}'(x, y, z + \Delta z) - \tilde{u}'(x, y, z - \Delta z)}{\Delta z^2}.
\]

The first- and second-order spatial derivatives for \(\tilde{\theta}\) are calculated similarly to those of \(\tilde{u}\). The nonlinear products (e.g., \(\tilde{\omega} \times \tilde{u}\) and \(\tilde{u}\tilde{\theta}\)) are calculated in the physical space (dealiasing is done by padding using the 3/2 rule). The modified pressure \((\tilde{p}^*)\) is solved numerically from the Poisson equation obtained by applying Eq. (2.7) to the divergence of Eq. (2.30), yielding

\[
\frac{1}{\rho_0} \nabla^2 \tilde{p}^{*,t} = \nabla \cdot \left[ \Gamma^t - \frac{1}{3} \text{RHS}_u^{t-\Delta t} \right],
\]

where \(\Gamma^t = \text{RHS}_u^t + (1/\rho_0)\nabla \tilde{p}^{*,t}\) can be calculated using known resolved variables (\(\tilde{u}'\) and \(\tilde{\theta}'\)). The spatial derivatives for \(\tilde{p}\) are calculated similarly to those of \(\tilde{u}\). So far we have obtained numerical representations for all terms in Eqs. (2.18), (2.21), and (2.22).
The concentration equation is discretized using finite-volume approach, with the concentration field (\( \tilde{C} \)) located on the same grid of horizontal velocity components (see details in Chamecki et al. (2008) [80]). The resolved concentration flux term is calculated as

\[
- \nabla \cdot (\tilde{u} \tilde{C})^t(x, y, z) = \\
\frac{1}{\Delta x} [\tilde{u}^t(x - (\Delta x/2), y, z)\tilde{C}^t(x - (\Delta x/2), y, z) \\
- \tilde{u}^t(x + (\Delta x/2), y, z)\tilde{C}^t(x + (\Delta x/2), y, z)] \\
+ \frac{1}{\Delta y} [\tilde{v}^t(x, y - (\Delta y/2), z)\tilde{C}^t(x, y - (\Delta y/2), z) \\
- \tilde{v}^t(x, y + (\Delta y/2), z)\tilde{C}^t(x, y + (\Delta y/2), z)] \\
+ \frac{1}{\Delta z} [\tilde{w}^t(x, y, z - (\Delta z/2))\tilde{C}^t(x, y, z - (\Delta z/2)) \\
- \tilde{w}^t(x, y, z + (\Delta z/2))\tilde{C}^t(x, y, z + (\Delta z/2))],
\]

where horizontal velocity components (\( \tilde{u} \) and \( \tilde{v} \)) as well as the concentration (\( \tilde{C} \)) at grid volume interfaces are obtained using the bounded third-order upwind interpolation scheme SMART [107]. So far we have obtained numerical representations for all terms in Eqs. (2.19) and (2.23).

### 2.2.3 Domain and Boundary Conditions

The lateral boundary conditions for velocity and potential temperature fields are periodic, which also implies periodic lateral boundary conditions for the modified pressure field. In Chapters 3–5, the domain of interest is confined to the canopy roughness sublayer \((z/h \lesssim 3)\), where \(h = 2.1 \text{ m} \) is the canopy height. The vertical domain, \(L_z = 10h\), is discretized as 120 grid points, so that the canopy is resolved as 12 vertical layers. The no-stress top boundary condition \((\partial \tilde{u}/\partial z = \partial \tilde{v}/\partial z = 0 \text{ and } \tilde{w} = 0 \text{ at } z = L_z)\) assumes no momentum exchange between the bottom 21 m of the atmosphere and the region above. However, this unrealistic assumption is not expected to have a significant impact on the turbulence statistics within the roughness sublayer [108]. This expectation is evaluated in Chapter 3 by comparing velocity statistics with results from a simulation using a larger vertical domain \((L_z = 20h)\). The underlying ground beneath the plants is modeled as a rough-wall boundary. The model provides the wall stress \((\tau_w)\) using the test-filtered horizontal
velocity components \((\hat{u} \text{ and } \hat{v})\) at the first vertical grid level \((z_1 = \Delta z/2)\),

\[
\tau_w(x, y) = -\left(\frac{\kappa}{\ln(z_1/z_0)}\right)^2 \left[\hat{u}^2(x, y, z_1) + \hat{v}^2(x, y, z_1)\right],
\]

where \(\kappa = 0.4\) is the von Kármán constant, and \(z_0 = 0.01\) m is the roughness length. Then \(\tau_w\) is partitioned into streamwise and spanwise directions (see detail in Bou-Zeid et al. (2005) [78]). The top and bottom boundary conditions for the modified pressure \((\tilde{p}^*)\) can be obtained from applying boundary conditions of \(\tilde{u}\) to the vertical component of Eq. (2.18), yielding

\[
\frac{1}{\rho_0} \frac{\partial \tilde{p}^*}{\partial z} = -\left(\frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z}\right) \text{ at } z = 0, L_z.
\]

For concentration, the outflow top boundary condition assumes that particles do not settle back to the bottom 21 m of the atmosphere \((\partial \tilde{C}/\partial z = 0 \text{ at } z = L_z)\). This is a good approximation for dispersion of particles within a few tens of canopy heights downwind from the source. The ground is modeled as a fully absorbent bottom boundary, using a prescribed reference concentration \((C_r = 0)\) at a reference height \((z_{0,c} = z_0)\). The model provides the concentration flux \((\Phi)\) between the ground and the atmosphere (concentration at the first grid level, \(\tilde{C}(x, y, z_1)\)) based on the flux-profile relationship proposed by Chamecki et al. (2007) for neutral conditions [86],

\[
\Phi(x, y) = -w_s \tilde{C}(x, y, z_1) \left(\frac{1}{\Gamma - (z_1/z_{0,c})^{-\gamma}}\right),
\]

where \(\gamma = (w_s Sc)/(\kappa u^*)\) is a measure of the relative importance of gravitational settling (characterized by settling velocity, \(w_s\)) and turbulent transport (characterized by friction velocity, \(u^*)\), and \(Sc = 0.5\) is determined from LES results for passive scalars under neutral conditions [92].

In Chapter 6, the domain of interest is the entire ABL (capped by a strong temperature inversion), and the ABL height \(z_i \lesssim 1000\) m (Table 6.2) is determined as the location of minimum heat flux. Coriolis force is neglected, and the flow is driven by a constant geostrophic wind at the top of the domain \((\tilde{u} = U_g, \tilde{v} = V_g, \text{ and } \tilde{w} = 0 \text{ at } z = L_z)\), making the region above and just below the temperature inversion different from the true ABL. However, this unrealistic representation is unlikely to affect the flow field within the bottom 20% of the ABL (the atmospheric
surface layer), where results are used to evaluate the theoretical model in Chapter 6. The vertical domain, $L_z = 1500$ m, is discretized as 500 grid points, so that the grid spacing ($\Delta z = 3$ m) is greater than the canopy height ($h = 1$ m). Therefore the canopy is modeled as a rough wall [79,81],

$$
\tau_w(x, y) = -\left[\frac{K}{\ln \left(\frac{z_1-d_0}{z_0}\right)} - \psi_m \left(\frac{z_1}{L_O}\right)\right]^2 \left[\hat{u}^2(x, y, z_1) + \hat{v}^2(x, y, z_1)\right],
$$

(2.43)

where $d_0$ is the displacement height, and $z_0$ is the roughness length. For bare ground, $d_0 = 0$ and $z_0 = 0.01$ m; for canopy, $d_0 = 3h/4$ and $z_0 = h/8$. The function $\psi(z_1/L_O)$ is determined as,

$$
\psi(z_1/L_O) = \int_{z_0/L_O}^{z_1/L_O} \frac{[1 - \phi_m(\zeta)]}{\zeta} d\zeta / \zeta,
$$

(2.44)

where the flux-profile function $\phi_m(\zeta) = (1 - 15.2\zeta)^{-1/4}$, $\zeta = z/L_O$ is given for unstable conditions (the Obukhov length $L_O < 0$) [82]. The top and bottom boundary conditions for the potential temperature field is zero-gradient ($\partial \tilde{\theta} / \partial z = 0$ at $z = L_z$) and a prescribed constant vertical heat flux ($q = \bar{w} \bar{\theta}^* e_z$ at $z = 0$), respectively, where $e_z$ is the unit vector in the vertical direction. Ignoring the local buoyant force, the top and bottom boundary conditions for the modified pressure ($\tilde{p}^*$) are given by Eq. (2.41). For concentration, the outflow top boundary condition ($\partial \tilde{C} / \partial z = 0$ at $z = L_z$) is a good approximation because almost no particles penetrate through the ABL height and reach the domain top. The transport of particles in the upper half of the ABL may be unrealistic, but these particles are unlikely to settle back to the atmospheric surface layer within a few kilometers downwind from the source field. The unrealistic representation of the flow field above and just below the temperature inversion is not expected to have a significant impact on the dispersion of particles within the atmospheric surface layer, where results are used to evaluate the theoretical model in Chapter 6. The concentration flux ($\Phi$) between the bottom boundary and the atmosphere is modeled as,

$$
\Phi(x, y) = -\frac{1}{\Omega(z_1/L_O)} w_s \frac{\tilde{C}(x, y, z_1) - C_r \left(\frac{z_1-d_0}{z_{0,c}-d_0}\right)^{-\gamma}}{1 - \left(\frac{z_1-d_0}{z_{0,c}-d_0}\right)^{-\gamma}},
$$

(2.45)

where $C_r$ is a reference concentration at a reference height, $z_{0,c}$. For bare ground,
\( C_r = 0, \) \( z_{0,c} = z_0; \) for canopy, \( C_r = C_0, \) \( z_{0,c} = d_0 + z_0. \) The stability correction, \( \Omega(\zeta) \) is given by Chamecki et al. (2007) [86].

So far we have obtained all boundary conditions for flow variables as well as top and bottom boundary conditions for the concentration field. For this entire work, the upwind and downwind boundary conditions for \( \bar{C} \) are zero-concentration inflow (\( \bar{C} = 0 \) at \( x = 0 \)) and outflow (\( \partial \bar{C}/\partial x = 0 \) at \( x = L_x \)), respectively. The spanwise boundary conditions are outflow (\( \partial \bar{C}/\partial y = 0 \) at \( y = 0, L_y \)) for point-source release in Chapters 3–5 and periodic for spanwise-infinite area-source release in Chapter 6.

### 2.3 Experimental Data and Model Evaluation Strategies

#### 2.3.1 Turbulence Statistics

LES results of turbulence statistics, mean particle concentration, and mean ground deposition rate obtained in Chapters 3–4 are evaluated against data obtained during a spore release and recapture experiment conducted in a large, flat mature maize field near Mahomet, Illinois (see detail in Gleicher et al. (2014) [4]). The experimental site was 120 m from the south edge and 500 m from the west edge of the field. The rows of maize were oriented in the north-south direction, with row spacing of 0.76 m. The wind direction was almost aligned with the rows of fully grown maize on 10 July 2011, when the canopy height was 2.1 m, and the one-sided leaf area index (LAI) was 3.3. Sonic anemometers were placed at five heights \( (z/h = 1/3, 2/3, 1, 4/3, \) and \( 5/3) \) to measure three-dimensional instantaneous velocity components at a sample frequency of 20 Hz. The fairly strong wind speeds, combined with small heat fluxes, yield a 7.5 hour period of statistical stationary turbulence during 0930–1700 CDT, 10 July 2011, providing good statistical sampling for turbulence statistics up to the third order and momentum fluxes carried by strong events [59].

The period is characterized by a friction velocity, \( u_* = \left[ -(\bar{w}'w')_h \right]^{1/2} = 0.51 \) m s\(^{-1}\), where the subscript \( h \) indicates the value at canopy top \( (z = h). \) Classical data obtained by Wilson et al. (1982) [1] on 2 and 4 August 1977 using split-film anemometers in a large flat mature maize field similar to that near Mahomet, Illinois were shown as a consistency check for turbulence statistics up to the second order.
Evaluation of velocity statistics consists of profiles of statistics up to the third order and momentum fluxes transported by strong events. For profiles of turbulence statistics (e.g., Figs. 3.1 and 4.3), height is normalized by the canopy height \((h)\), while velocity statistics are normalized by the corresponding orders of friction velocity \((u_*)\). Following the standard practices in LES studies, the mean momentum flux \((u'w')\) and consequently the friction velocity are determined using the resolved and SGS parts. However, standard deviations and skewness of velocity components are determined based only on the resolved scales. The momentum fluxes transported by strong events are investigated using quadrant analysis proposed by Lu and Willmarth (1973) [109] (e.g., Figs. 3.2 and 4.4). The vertical momentum flux is decomposed into four quadrants. Events in the first quadrant \((u' > 0, w' > 0)\) are outward interactions, events in the second quadrant \((u' < 0, w' > 0)\) are ejections, events in the third quadrant \((u' < 0, w' < 0)\) are inward interactions, and events in the fourth quadrant \((u' > 0, w' < 0)\) are sweeps [110]. Note terms ejections and sweeps are defined using velocity fluctuations, and are different from their classical definitions associated with the movement of air parcels. This analysis provides the fraction of momentum carried by a certain category of events \(H\) times stronger than the mean momentum flux, where \(H = |u'w'|/|u'w'|\) is known as the “hole size” [109]. In this analysis, the SGS component of the vertical momentum flux is excluded.

**2.3.2 Dispersion of Particles**

During the 30-minute spore release experiment (1143–1213 CDT, 10 July 2011), blue, yellow, and red Lycopodium spores were released simultaneously from artificial continuous sources placed at three different heights \((z/h = 1, 2/3, \text{and } 1/3;\) represented by pentagram, triangle, and circle in Fig. 3.3, respectively) [4]. The Lycopodium spores have a mean density, \(\rho_p = 1.15 \text{ g cm}^{-3}\), and a mean Stokes diameter, \(d_{St} = 23.6 \mu \text{m}\) [111], yielding a mean settling velocity in still fluid,

\[
w_s = (\rho_p - \rho_a)gd_{St}^2/(18\mu) = 1.94 \text{ cm s}^{-1}.
\]

Here \(\rho_a \ll \rho_p\) is the density of air, \(\mu = 1.8 \times 10^{-5} \text{ Kg m}^2 \text{ s}^{-1}\) is the dynamic viscosity of air, and \(g = 9.81 \text{ m s}^{-2}\) is the gravitational acceleration. The weight of Lycopodium spores \((m)\) was recorded at the beginning and end of the experiment.
and used to determine the total number of spores released during the 30-minute experiment, \(N_Q = m N_0\). Here \(N_0 = 1/(\pi \rho_p d_p^3/6) = 4.71 \times 10^7\) spores g\(^{-1}\) is the number of spores per gram estimated by assuming Lycopodium spores to be spheres with a mean geometric diameter, \(d_p = 32.8\ \mu \text{m}\) [112]. Nine poles (numbered 1–9) were deployed in a 3 × 3 grid, as illustrated in Fig. 3.3. The centre row and the source location form a straight line parallel to the row of maize, and parallel side rows are 0.76 m away from the centre row. The three columns of poles were placed at 2, 4, and 8 m downwind from the source. Rotorods were placed on each pole at the same five heights as those of sonic anemometers (crosses in Fig. 3.3), and two sampling rods were mounted on each rotorod box to collect spores, forming a three-dimensional sampling array containing 90 samplers of mean spore concentration. During the 30-minute experiment (\(T = 30\ \text{min} = 1800\ \text{s}\)), each rod sampled an air volume,

\[
V_R = \pi d_R A_R \times \text{RPM} \times f_R \times T \sim 0.1\ \text{m}^3. \tag{2.47}
\]

Here \(d_R = 8.6\ \text{cm}\) is the diameter of the rotorod arm, \(A_R = 0.25\ \text{cm}^2\) is the surface area of the sampling rods mounted on each end of the rotorod arm, RPM is the number of rotation per minute, and \(f_R\) is the fraction of time sampled. Using the counts of spores collected on individual sampling rods, \(N_R\), we obtain a 3-D array of the normalized mean spore concentration,

\[
\overline{C}/Q = (N_R/V_R)/(N_Q/T), \tag{2.48}
\]

which is used to evaluate LES results of mean particle concentration field (\(\overline{C}\)) normalized by the point-source strength (\(Q\)).

Evaluation of mean particle concentration consists of vertical profiles at individual pole locations (e.g., Fig. 3.5) and statistical metrics describing overall model performance (e.g., Table 3.2). We use three metrics that have been commonly used in the evaluation of dispersion models [113]. The geometric mean bias,

\[
\text{MG} = \exp \left[ \frac{1}{N} \sum_{i=1}^{N} \left( \ln(\overline{C}_i/Q)_{\text{obs}} - \ln(\overline{C}_i/Q)_{\text{LES}} \right) \right], \tag{2.49}
\]

measures the mean shift of LES results from observations (denoted by subscripts “LES” and “obs”, respectively), where \(N\) is the sample size. Compared with arithmetic mean bias, the geometric mean bias takes the advantage of weighing
underestimation and overestimation equally, which is particularly important for this work, because the observed values of mean concentration spread over two orders of magnitude (see Figs. 3.4 and 3.5). The geometric variance,

$$VG = \exp \left[ \frac{1}{N} \sum_{i=1}^{N} \left( \ln \left( \frac{C_i}{Q} \right)_{\text{obs}} - \ln \left( \frac{C_i}{Q} \right)_{\text{LES}} \right)^2 \right],$$  \hspace{1cm} (2.50)

and the fraction of predictions within a factor of two of observations,

$$\text{FAC2} = \text{fraction of data that satisfy } 0.5 \leq \frac{(C/Q)_{\text{obs}}}{(C/Q)_{\text{LES}}} \leq 2.0,$$ \hspace{1cm} (2.51)

measure the random scattering of LES results from observations. A perfect dispersion model corresponds to $MG = 1$, $VG = 1$, and $\text{FAC2} = 100\%$. Chang and Hanna (2004) suggest that a dispersion model should be considered good if the mean bias is within $\pm 30\%$ of the mean ($0.7 < MG < 1.3$), the random scatter is within a factor of two of the mean ($VG < 1.6$), and $\text{FAC2} > 50\%$ [9].

Measurements of mean ground deposition rate were obtained by placing glass slides (with surface area $A_S = 3.2 \text{ cm}^{-2}$) along the centre line of the grid at $-1, 1, 2, 3, 4, 5, 6, 7,$ and $8 \text{ m}$ downwind from the source (squares in Fig. 3.3). Using the counts of spores ($N_S$) deposited on individual slides, we obtain a 1-D array of the normalized mean ground deposition rate,

$$\Phi_G/Q = (N_S / A_S) / N_Q,$$ \hspace{1cm} (2.52)

which is used to evaluate LES results of mean ground deposition rate ($\Phi_G$) normalized by the point-source strength ($Q$). The evaluation is conducted by plotting the normalized mean ground deposition rate against the downwind location of slides (Fig. 3.6). The measurements of mean ground deposition rate were less reliable than those of mean concentration due to small sampling area as well as the difference between glass slides and the soil surface.
Chapter 3  
Large-Eddy Simulation of Turbulence and Particle Dispersion Inside the Canopy Roughness Sublayer

3.1 Introduction

Knowledge of atmospheric dispersion of small particles such as fungal spores released inside plant canopies is important for a number of practical applications. Many common plant diseases are spread by aerial dispersal of pathogenic fungal spores [28]. Cereal rusts, for example, are one of the most important diseases worldwide [31]. The repeating cycle of a rust disease epidemic requires spores to be released from infected host surfaces inside the canopy, escape from the canopy region, and deposit on fresh host tissue in environmental conditions favorable to cause infection [15,114]. Viable spores must escape the canopy in order to spread an epidemic widely and rapidly; otherwise they deposit on the ground and canopy elements within a few meters of the source [114]. The product of release rate and escape fraction is commonly used to quantify emission of spores from canopies in plume models that predict spatial distribution of spores deposited downwind and the spread of spores between fields, farms, and crop-growing regions [37,42]. The fraction of spores that escape the canopy increases with wind speed, turbulence level, and release height [37,115]. Infections caused by rusts, like those of many plant diseases, are
usually first observed in the lower to middle canopy region of a crop where they spread horizontally to nearby plants (within about one meter) while spreading vertically at a slower rate. However, once infections reach foliage at the canopy top, the dynamics of disease spread change dramatically as the spores released from the infections spread rapidly across the landscape [29]. Thus the escape of spores released from point sources inside the canopy and the follow-up growth of the spore plume above the canopy are critical components of the early stage of disease epidemics in crops, and are the focus of this study.

Escape fraction and the initial growth of the particle plume are determined by the characteristics of the turbulence in the canopy roughness sublayer, the region of the flow strongly modified by the presence of the plant canopy (extending from the ground to about three canopy heights [98]). Field experimental data obtained over horizontally dense and uniform crop canopies show that turbulence near the top of the canopy resembles the flow in a mixing layer rather than a boundary layer [47]. Instabilities similar to those in a mixing layer arise from the inflectional mean velocity profile with a shear maximum at canopy top, and determine the structure of coherent eddies. The dynamic interactions between the overlying flow and the canopy result in a complex turbulence field, characterized by fairly strong vertical heterogeneity, non-Gaussian velocity fluctuations, and highly organized motions with large integral time and length scales [48,59,98]. Turbulence statistics within the canopy roughness sublayer, such as the variance and skewness of velocity fluctuations, as well as the turbulent kinetic energy (TKE) budget are also similar to those in a mixing layer [47]. A theoretical treatment of dispersion in heterogeneous non-Gaussian turbulence fields is still lacking, and reliable estimates for the escape fraction of particles released within the canopy are unavailable.

Raupach et al. (1996) [47] proposed a canopy-mixing layer analogy in which the mixing length (calculated as the ratio between mean velocity and mean shear at canopy top) is used to scale coherent eddies, and the inverse of mixing length is used to represent the wave number of the fastest growing instability. A priori specification of mixing length enables use of first-order closure models [49], one- (or $K-U$) and two-equation (or $K-\epsilon$) models [116,117], and second-order closure models [4,50] to reproduce turbulence statistics inside a wide range of plant canopies. Challenges are associated with the highly empirical parameterization of mixing length that is difficult to model with a high degree of confidence. In addition, many applications
within plant canopies are dominated by near-field dispersion [59, 62], which is not a diffusive process and cannot be accurately modelled using eddy-diffusivity approaches [60].

The use of Lagrangian Stochastic models (LSMs) has been the preferred approach to study dispersion of scalars [63–65] and particles [37, 66, 67] inside plant canopies and to estimate spore escape fraction [4, 37, 115]. These models usually assume Gaussian turbulence statistics and require specification of vertical profiles of first- and second-order moments of velocity fluctuations and the Lagrangian timescale. Limited comparisons with field experimental data suggest that LSMs provide reasonable results for dispersion of particles released in the upper half of a canopy [66, 67]. However, the dispersion process inside canopies is influenced by intermittent strong gusts associated with non-Gaussian features in the probability density function (PDF) of streamwise and vertical velocity fluctuations [15, 99]. The inclusion of non-Gaussian statistics into LSMs of particle dispersion in canopy flows, on the other hand, has not improved predictions for mean concentration profiles [63, 103]. A comprehensive comparison between LSM predictions and experimental data of particle dispersion within and above a maize canopy clearly shows that model predictions are sensitive to the parameterization of the Lagrangian timescale, and that existing parameterization schemes do not provide accurate reproduction of the vertical dispersion [4].

Reynolds-averaged Navier-Stokes (RANS) models yield predictions of mean particle concentrations and ground deposition rates for particles released at the canopy top that are similar in accuracy to those produced by LSMs [118]. RANS approaches have the advantage that the velocity statistics are also calculated by the model, making them easily applicable to heterogeneous landscapes. Higher-order closure schemes proposed for RANS models require parameterization for terms in the turbulent flux budget, some of which are difficult to model and measure [119, 120]. Large-eddy simulation (LES) models are the best approach to reveal the complex structure of canopy flows [52]. Canopy-resolving LES models that parameterize the canopy as a drag field [52–57] predict profiles of mean velocity, mean Reynolds stress, TKE, and standard deviation of velocity fluctuations in good agreement with field experimental data. These studies (except for Shaw and Schumann (1992) [52]) also evaluated skewness of streamwise and vertical velocity fluctuations, showing an under-prediction of more than 50% for observations. Strong
events evaluated through quadrant analysis were not well reproduced by the LES either [95]. Increasing grid resolution induced negligible changes in the comparison for skewness and results of quadrant analysis [55,95]. It is unlikely that accounting for the effects of temperature stratification would reduce the underestimation of skewness, because the largest skewness values within the canopy were observed under neutral conditions [97]. Even the explicit inclusion of plant motion as a linear mode of vibration to represent the spatial and temporal characteristics of wave-like plant motions was unable to improve the prediction of skewness [96]. To date, the best reproduction of skewness by LES models was obtained for a maize canopy by considering the geometric structure of individual plants [55]. Nonetheless, the plant-scale approach has been unable to reproduce the strong events in the quadrant analysis of experimental data with sufficient accuracy [95].

The objectives of this work are to: (1) improve predictions of turbulent statistics and dispersion of particles inside the canopy roughness sublayer by refining the current approach to canopy-resolving LES, and (2) propose a theoretical model for dispersion of particles released from continuous point sources inside plants canopies. The parameterization of canopy effects is described in Section 3.2. Field measurements of velocity and aerial concentration and ground deposition of Lycopodium spores released from artificial point sources in a large cornfield are used to evaluate LES results in Section 3.3. The effects of source height and gravitational settling on escape fraction and the growth of particle plume are investigated in Section 3.4. Conclusions follow in Section 3.5.

### 3.2 Large-Eddy Simulations

#### 3.2.1 Model Description

The LES model employed to simulate turbulence and particle dispersion has been described in detail in Chamecki et al. (2009) [81] and has been used in a number of studies of particle dispersion in the atmospheric boundary layer [12,81,92,121]. The model solves the three-dimensional filtered momentum equation using a fully dealiased pseudo-spectral approach in horizontal directions and a second-order centered finite-difference scheme in the vertical direction. The flow is driven by an imposed mean pressure gradient. Viscous effects are neglected in view of the very
large Reynolds number and the equations are closed using the Lagrangian scale-dependent dynamic Smagorinsky subgrid-scale (SGS) model [78]. Lateral boundary conditions are periodic. A no-stress boundary condition is imposed at the top boundary and a wall model is used to parameterize the bottom boundary condition at the soil surface beneath the plants. Buoyancy effects are not considered.

Particle dispersion is treated using an Eulerian approach. The conservation of particle concentration is discretized using a finite-volume scheme with a third-order bounded scheme for the advection term [80]. Following Chamecki and Meneveau (2011) [92], the advective velocity for the particle concentration field is approximated as the superposition of the instantaneous fluid velocity and a constant particle settling velocity (which represents the “mean drift” due to gravitational settling). Because only small Stokes numbers are considered in the simulations, the effect of particle inertia is neglected [12]. The SGS particle flux is modeled using an eddy-diffusivity approach and a constant SGS Schmidt number, $S_{\text{cSGS}} = 0$ [81]. The upwind, downwind, top, and bottom boundary conditions for the particle concentration field are specified as zero concentration inflow, outflow, outflow, and fully absorbent (parameterized using a wall model with specification of zero-concentration at $z = z_0$), respectively.

The LES model was refined to resolve the canopy region, where the effects of canopy on velocity and particle concentration fields are parameterized as terms in the momentum and particle conservation equations. The momentum equation for neutral conditions is written as [52],

$$\frac{\partial \tilde{u}}{\partial t} = -\tilde{u} \cdot \nabla \tilde{u} - \frac{1}{\rho} \nabla \tilde{p} - \nabla \cdot \tau + d,$$

(3.1)

where $\tilde{u}$ is the filtered velocity, $(1/\rho) \nabla \tilde{p}$ is the filtered pressure gradient force, and $\nabla \cdot \tau$ is the divergence of the SGS momentum flux. The drag force $d$ exerted by canopy elements on the airflow is modeled following the approach proposed by the pioneer LES study of Shaw and Schumann (1992) [52],

$$d = -C_d (aP) \cdot (|\tilde{u}| \tilde{u}).$$

(3.2)

Here, $C_d$ is the drag coefficient and $a$ is the leaf area density. The projection coefficient tensor $P = P_x e_x e_x + P_y e_y e_y + P_z e_z e_z$ is used to obtain the effective
leaf area density facing streamwise, spanwise, and vertical directions \((e_j\) is the unit vector in the \(j^{th}\) direction and \(x, y,\) and \(z\) are coordinates along the streamwise, spanwise, and vertical directions, respectively). Coefficients \(P_x, P_y,\) and \(P_z\) depend on the distribution of individual canopy elements (e.g., leaves and stems), their geometry (e.g., flat or round), and their instantaneous posture (e.g., angle and bending) \[67\]. The assumption of horizontally homogeneous canopy implies that \(a, P_x, P_y,\) and \(P_z\) are functions of height \((z)\) only, although the geometry and posture of plants in a canopy vary with time and space. Values of \(a, P_x, P_y,\) and \(P_z\) for the specific canopy of interest are provided in Section 3.2.2.

The treatment of \(C_d\) influences the accuracy of modeled turbulence statistics and structures, regardless of the turbulence closure scheme adopted \[122\]. For an isolated rigid cylinder in cross flow, \(C_d\) is approximately independent of Reynolds number \((Re)\) in the range \(10^2 < Re < 10^5\). The Reynolds number for flow past individual canopy elements is usually within this range. For a maize canopy, \(Re\) ranges between 110 and 5500 for a characteristic length scale \(L_v = 0.02\) m (stalk diameter and projected width of leaf) and velocities between 0.1 and 5 m s\(^{-1}\). Even though the interference of the wakes from various canopy elements can affect the dependence of \(C_d\) on \(Re\) \[49\], the effect of \(Re\) on \(C_d\) is assumed to be small compared to the effects of reconfiguration discussed below. Previous LES studies of forests \[52–54, 56, 57, 68\] and crop canopies \[55, 95, 96, 123\] typically treat \(C_d\) as a constant. However, field measurements of maize canopies \[1, 124\] suggest that \(C_d\) decreases with increasing height \((z)\) in the upper 1/3 of the canopy \((crosses and filled triangles in Fig. 5 of Brunet et al. 1994 Brunet1994BLM)\). Here it is assumed that the variations in \(C_d\) are caused by the reconfiguration of flexible canopy elements.

The reconfiguration mechanism represents the reaction of plants that favours the survival in flow-dominated habitats via a non-permanent, passive adaptive process that allows plants to minimize the increase in drag force with increasing velocity \[125\]. This mechanism has been observed for flowers \[126\], leaves \[127\], grasses \[128\], reeds \[129\], trees \[130, 131\], freshwater plants \[132, 133\], and seaweeds \[134, 135\]. The effect of reconfiguration has been described empirically by modifying the quadratic drag law \(|d| \propto U^2\) that introduces the Vogel number \(B\) to the power exponent and yields \(|d| \propto U^{2+B}\) \[125, 135\]. The negative Vogel number \((B < 0)\), named after Steven Vogel \[125\], describes a slower increase of drag with velocity due to
reconfiguration. This slower increase of drag with velocity can also be modeled by maintaining the quadratic dependence of drag on velocity implied by Eq. (3.2) and introducing a velocity-dependent drag coefficient $C_d \propto U^B$. Theoretically the dependence of drag on the rigidity of a flexible body changes $C_d$ from a constant to a function of Cauchy number ($Ca \propto U^2$; see definition given by Eq. (4.2)) that measures the relative importance of the inertia force of the flow and the bending rigidity of canopy elements [136]. For one-dimensional linear elastic bending, theoretical models based on force balance between posture-dependent drag and internal resistance successfully reproduced laboratory measurements of $C_d$ as a function of $Ca$ [3,136]. Values of $B$ vary for different regimes of Cauchy number. In the asymptotic low Cauchy number regime, $B \approx 0$ as reconfiguration is negligible. In the asymptotic high Cauchy number regime (strong reconfiguration), dimensional analysis suggests $B = -2/3$ and $-4/3$ for one- and two-dimensional linear elastic bending and $B = -2N/(2N + 1)$ for one-dimensional non-linear elastic bending, where $N = 0, 1$, and $\infty$ for rigid ($B = 0$), linear elastic ($B = -2/3$), and perfect plastic ($B = -1$) bending, respectively [2,137]. In this study the general expression $C_d = (\|\tilde{u}\|/A)^B$ is adopted, where $A$ is a velocity scale related to plant geometry and rigidity. The values of $A$ and $B$ used here are discussed in Section 3.2.2.

To simulate dispersion of the particle cloud, the conservation equation for the filtered particle concentration $\tilde{C}$ is written as,

$$\frac{\partial \tilde{C}}{\partial t} = - (\tilde{u} - w_e e_z) \cdot \nabla \tilde{C} - \nabla \cdot \pi^C - S_p + q_{src}, \quad (3.3)$$

where $w_e$ is the gravitational settling velocity, $\pi^C$ is the SGS particle concentration flux, and $q_{src} = Q/\Delta x \Delta y \Delta z$ is the local particle release rate (represented as the strength of the point source $Q$ well-mixed in a single grid box). The rate of particle deposition on canopy elements, $S_p$, is parameterized using a modified version of the model described by Aylor and Flesch (2001) [67], in which $S_p$ combines deposition on horizontal surfaces due to gravitational settling and on vertical surfaces due to impaction. A detailed discussion of the deposition model can be found in Appendix A.
3.2.2 Simulation Setup

LES runs were performed to study turbulence and particle dispersion inside and above a maize canopy. The simulation domain is a box with $L_x \times L_y \times L_z = 20h \times 20h \times 10h$, discretized using $84 \times 84 \times 120$ grid points respectively (here $h$ is the canopy height). The modeled canopy occupies the entire horizontal domain and the first 12 vertical layers. The vertical domain size of $10h$ is expected to be sufficient for LES to capture scales of motions that affect turbulence structures inside the canopy roughness sublayer [108]. Note that the no-stress boundary condition at the top of the domain is not realistic at this height, but this detail is not expected to impact statistics within the roughness sublayer. This expectation is evaluated by comparing statistics of the velocity field with results for an additional simulation using a $40h \times 40h \times 20h$ domain discretized on a $168 \times 168 \times 240$ grid (i.e. a domain twice as large in each dimension using the same grid spacing). A roughness length of $z_0 = 0.01$ m was used for the lower boundary condition wall model in all simulations. Particle dispersion was simulated for 1.2 hours in each case study. Prior to each run, a spin-up time of 18 minutes (much larger than the eddy-turn-over time, $\sim 1$ minute, calculated as the vertical domain size divided by friction velocity) was used to allow the velocity profile to adjust to the presence of the canopy and the turbulence to reach a statistically steady state. The analysis of results is based on the last hour of each LES case study, and thus approximates statistically steady-state conditions for the concentration field.

The model for the drag force (Eq. (3.2)) requires specification of the vertical distribution of leaf area density $a(z)$ and the projection of leaf area index (LAI) in each direction. Measurements in a dense maize canopy [1] provide values of $a(z)$ shown in Table 3.1 and suggest that $P_x = P_y$, while the the geometric structure of maize canopy provided by Bouvet et al. (2007) [138] suggests that $P_z = 0.44$ (and thus $P_x = P_y = 0.28$). The drag coefficient ($C_d$) can be estimated by fitting data to the mean momentum equation [122,139–141]. Wilson et al. (1982) [1] reported $C_d = 0.07$ for the model $d = C_d a(z)|u|u$, equivalent to $C_d = 0.07/P_x = 0.25$ for the model Eq. (3.2). Here field experimental data obtained in a maize field of similar structure [4] and the approach of Cescatti and Marcolla (2004) [140] were used to estimated $C_d$. Fitting a constant drag coefficient to the data yields $C_d = 0.28$, consistent with $C_d = 0.25$ reported by Wilson et al. (1982) [1].
<table>
<thead>
<tr>
<th>$z/h$</th>
<th>$a(z)/\text{LAI} \text{[m}^{-1}]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 – 0.15</td>
<td>0.34</td>
</tr>
<tr>
<td>0.15 – 0.30</td>
<td>0.75</td>
</tr>
<tr>
<td>0.30 – 0.45</td>
<td>1.36</td>
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<tr>
<td>0.45 – 0.60</td>
<td>1.50</td>
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<tr>
<td>0.60 – 0.75</td>
<td>1.61</td>
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<tr>
<td>0.75 – 0.90</td>
<td>1.50</td>
</tr>
<tr>
<td>0.90 – 1</td>
<td>0.43</td>
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</tbody>
</table>

Table 3.1. Two-sided leaf area density ($a(z)$) normalized by one-sided leaf area index (LAI) for heights ($z$) normalized by canopy height ($h$) for cornfield measured by Wilson et al. (1982) [1].

$C_d = 0.25$ instead of $C_d = 0.28$ induces negligible changes in LES results. Fitting the power-law dependence $C_d = (\langle |\tilde{u}| \rangle / A)^B$ to the data yields $A = 0.29 \text{ m s}^{-1}$ and $B = -0.74$ (see Appendix B). The Vogel number ($B$) is within the theoretical range $-1 < B < -2/3$ for one-dimensional linear elastic bending in the regime of weak-to-strong reconfiguration [11,136]. This value ($B = -0.74$) is similar to the experimental value $B = -0.71$ reported by Harder et al. (2004) [129] for giant reed *Arundo Donax* under flow rates $u \gtrsim 1.5 \text{ m s}^{-1}$. Both *Arundo Donax* and maize are from the *Gramineae* family, and have similar structure. Two different models for the drag coefficient were used: (1) $C_d = \text{constant} = 0.25$ as usually adopted in LES of canopy flows, and (2) $C_d = (\langle |\tilde{u}| \rangle / A)^B$, where $A = 0.29 \text{ m s}^{-1}$ and $B = -0.74$, to account for the drag reduction due to plant reconfiguration.

Two sets of simulations were performed with different goals. In the first set designed for comparison with the field experimental data, six simulations were carried out using the two drag coefficient models described above and three source heights ($z_{src}/h = 1, 2/3, \text{and } 1/3$). The simulations were designed to reproduce measurements during a particle release experiment conducted in a large maize field described in detail by Gleicher et al. (2014) [4]. The relevant features of the experiment are introduced below and in Section 3.3. Data used here were collected on 10 July 2011, when the canopy height was $h = 2.1 \text{ m}$ and the one-sided leaf area index was LAI = 3.3. The period is characterized by a friction velocity $u_* = \left[-(\langle u'w' \rangle)_h\right]^{1/2} = 0.51 \text{ m s}^{-1}$, where the subscript $h$ indicates the value at $z = h$ ($\langle |v'w'| \rangle$ is neglected here because it is three orders of magnitude smaller than $|\tilde{u}'w'|$).
in both field and LES data). Lycopodium spores with settling velocity \( w_s = 1.94 \text{ cm s}^{-1} \) were continuously released during a period of 30 minutes from point sources placed at three heights: \( z_{src}/h = 1/3, 2/3, \) and 1. The simulation used observed values for canopy height, leaf area index, settling velocity, and friction velocity. Due to the low value \( w_s/u_\star \approx 0.04 \), the Lycopodium spores used in the experiment are considered light particles. The second set of simulations was designed to provide a database for analysis of plume statistics and investigation of theoretical model. This set contained 19 simulations using \( C_d = (|\tilde{u}|/A)^B \) (\( A = 0.29, B = -0.74 \), the model that reproduces field experimental data well, see Section 3.3.1 and Section 3.3.2 for details). Ten simulations were for light particles \( (w_s/u_\star \approx 0.04) \) released at \( 1/4 \leq z_{src}/h \leq 1 \) and the other nine were for heavier particles \( (w_s = 10 \text{ cm s}^{-1} \) and \( w_s/u_\star \approx 0.2 \), which would correspond to larger particles such as pollen grains) released at \( 1/3 \leq z_{src}/h \leq 1 \). The increment \( \Delta z_{src}/h = 1/12 \) was used for both light and heavy particles.

### 3.3 Evaluation of LES Results

#### 3.3.1 Evaluation of Velocity Statistics

In this section turbulence statistics from LES are compared to field experimental data obtained from sonic anemometers deployed at five heights within the canopy roughness sublayer above a large maize field: 0.7 m \( (z/h = 1/3) \), 1.4 m \( (z/h = 2/3) \), 2.1 m \( (z/h = 1) \), 2.8 m \( (z/h = 4/3) \), and 3.5 m \( (z/h = 5/3) \). Statistics from the field experiment are computed using the entire 7.5 hour period of steady turbulence (0930–1700 CDT, 10 July 2011), yielding good statistical sampling for most quantities of interest as seen in Fig. 3.1. As discussed in Chamecki (2013) [59], this period corresponds to over 25,000 integral timescales, allowing good sampling of extreme events and reliable estimates of skewness. In addition, 30-minute averages corresponding to the time of the spore release experiment (1143–1213 CDT, 10 July 2011) and the classic data obtained by Wilson et al. (1982) [1] on 2 and 4 August 1977 [142] are also shown. The good agreement between our data and the split-film anemometer of Wilson et al. (1982) [1] in the profiles of normalized first- and second-order statistics demonstrate the capabilities of sonic anemometers for making measurements inside the maize canopy roughness sublayer (dots and circles...
compared with crosses in Fig. 3.1a–f). Following standard practices in LES studies, the mean stress $\overline{u'w'}$ (and consequently the friction velocity) is determined using the resolved and SGS parts. However, standard deviations and skewness of velocity components are determined based only on the resolved scales.

In addition to vertical profiles of turbulence statistics, mechanisms of momentum transport inside the canopy are investigated following the approach proposed by Lu and Willmarth (1973) [109] that decomposes the vertical momentum flux into four quadrants. Events in the first quadrant ($u' > 0, w' > 0$) are outward interactions, events in the second quadrant ($u' < 0, w' > 0$) are ejections, events in the third quadrant ($u' < 0, w' < 0$) are inward interactions, and events in the fourth quadrant ($u' > 0, w' < 0$) are sweeps [110]. Given a hole size $H = |u'w'|/|\overline{u'w'}|$, $S_{i,H}$ indicates the momentum flux $u'w'$ carried by events in the $i^{th}$ quadrant stronger than $H$ times the mean momentum flux ($|u'w'|/|\overline{u'w'}| > H$), $S_{i,H}^f = S_{i,H}/u'w'$ indicates the fraction of momentum flux carried by these events, and $S_H^f = \Sigma_{i=1}^4 S_{i,H}^f$ indicates the fraction of momentum flux carried by events stronger than $H$ times the mean momentum flux in all four quadrants. In this analysis, the SGS component of the vertical momentum flux is excluded.

The performance of LES using $C_d = \text{constant}$ is similar to that obtained by Yue et al. (2007) [55], showing acceptable reproduction of turbulence statistics up to the second order. Nevertheless, large underestimation of the positiveness of $\text{Sk}_u$, the negativeness of $\text{Sk}_w$, and the ratio between the stress fraction carried by sweeps and ejections $S_{4.0}/S_{2.0}$ are predicted inside the canopy (dash lines in Fig. 3.1). Accounting for the effect of reconfiguration ($C_d = (|\overline{u}|/A)^B$) induces negligible changes in the predictions of $-\overline{u'w'}/u_*^2$, $\sigma_u/u_*$, $\sigma_v/v_*$, and $\sigma_w/u_*$. However, this approach eliminates the overprediction of $\overline{u}/u_*$, reduces the underprediction of $\text{Sk}_u$ and $S_{4.0}/S_{2.0}$ from 60% to 5%, and reduces the underprediction of $\text{Sk}_w$ from 60% to 20% (black solid lines compared with dash lines in Fig. 3.1). Note that the improvements in the predictions of the latter three statistics are most apparent in the upper half of the canopy (Fig. 3.1g, i, c), where the downward momentum flux is significant ($-\overline{u'w'}/u_*^2 = \overline{u'w'}/\overline{u'w'}h \gtrsim 0.1$, see Fig. 3.1h). The changes in $S_{4.0}/S_{2.0}$ suggest that reconfiguration may alter the mechanism of momentum transfer without significantly modifying the vertical profile of mean momentum flux.

The distribution of momentum flux events using the quadrant-hole analysis for
Figure 3.1. Comparison of LES results and field experimental data against normalized height \((z/h)\) for: normalized mean wind \((\bar{u}/u_\star; \text{a})\), normalized mean Reynolds stress \((-u'w'/u_\star^2; \text{b})\), ratio between momentum fluxes carried by sweeps and ejections \((S_{4,0}/S_{2,0}; \text{c})\), normalized standard deviation of streamwise \((\sigma_u/u_\star; \text{d})\), spanwise \((\sigma_v/u_\star; \text{e})\), and vertical \((\sigma_w/u_\star; \text{f})\) velocity fluctuations, and skewness of streamwise \((Sk_u; \text{g})\), spanwise \((Sk_v; \text{h})\), and vertical \((Sk_w; \text{i})\) velocity fluctuations. Black and grey lines indicate results given by LES conducted for vertical domain sizes of \(10h\) and \(20h\), respectively. Dash and solid lines indicate results given by LES using \(C_d = \text{constant}\) and \(C_d = (|\tilde{u}|/A)^B\), respectively. Dots with errorbars indicate average and standard deviation for 30-minute intervals of data obtained during 0930–1700 CDT on 10 July 2011, circles indicate data obtained during 1143–1213 CDT on 10 July 2011, and crosses indicate data obtained by Wilson et al. (1982) [1]. The canopy type and structure are similar in both datasets, and the model represents systems of different geometry and flow conditions with length scales normalized by canopy height \((h)\) and velocity scales normalized by friction velocity \((u_\star)\).
LES results and field experimental data at $z/h = 2/3$ are compared in Fig. 3.2. Treating $C_d$ as a constant underestimates $S_H^f$ at large values of $H$, implying that strong events are dampened by the large resulting drag forces (the dash line in Fig. 3.2e). Sweeps ($S_H^f$) are significantly underestimated over the entire range of $H$ investigated, while ejections ($S_H^f$) are overestimated at small values of $H$ (dash lines in Fig. 3.2d, a). These results are consistent with those presented by Yue et al. (2007) [95]. Treating $C_d = (|\bar{u}|/A)^B$ eliminates the overestimation of ejections and reduces the underestimation of sweeps and $S_H^f$ from 40% to 5% (black solid lines compared with dash lines in Fig. 3.2a, d, e). Considering the effect of the plant reconfiguration yields a much larger fraction of strong events, because canopy elements tend to align more with wind direction during strong momentum flux events, reducing the drag.

The shallow vertical domain used in the simulations presented here could cause deviations between numerical results and observational data. Increasing the vertical domain size from $10h$ to $20h$ leads to 2% decrease of $\bar{\pi}/u_*$ and 3% increase of $-\bar{u}\bar{w}/u_*^2$, $\sigma_u/u_*$, and $\sigma_v/u_*$ above the canopy (grey solid lines compared with black solid lines in Fig. 3.1a, b, d, e). The small improvement in the predictions of $\sigma_u/u_*$ and $\sigma_v/u_*$ suggests that their underestimation above the canopy could be caused in part by the shallow vertical domain, which prevents large eddies from being represented. The underestimation of $\sigma_u$ and $\sigma_v$ can cause underestimation of turbulent transport in corresponding directions. Increasing the vertical domain size also causes 2% increases of $Sk_u$ and $S_{4,0}/S_{2,0}$ (grey solid lines compared with black solid lines in Fig. 3.1g, c). The effects of altering the vertical domain size from $10h$ to $20h$ on the fraction of quadrant events at $z/h = 2/3$ are negligible (grey solid lines compared with black solid lines in Fig. 3.2). Overall, the influence of the domain height on the results is small and hence the choice of the shallower domain is adequate for the purpose of this study.

### 3.3.2 Evaluation of Particle Dispersion

Simulations of particle dispersion using the two models for the drag coefficient described above are conducted to reproduce the conditions during the field experiment. In the field experiment spores were released at $z_{src}/h = 1, 2/3,$ and $1/3$. Nine poles were deployed in a $3 \times 3$ grid, as illustrated in Fig. 3.3, where the centre
Figure 3.2. Comparison of LES results and field experimental data for fractions of momentum fluxes carried by ejections ($S_{1,H}^f$; a), outward interactions ($S_{1,H}^f$; b), inward interactions ($S_{3,H}^f$; c), sweeps ($S_{4,H}^f$; d), and their summation ($S_{H}^f$; e) against hole size ($H$) at $z/h = 2/3$. 

Lines and symbols are defined in Fig. 3.1.
Figure 3.3. Design of field experiment near Mahomet, Illinois. The canopy height \(h\) was 2.1 m on 10 July 2011. Point sources are represented by a pentagram for blue spores released at \(z_{src}/h = 1\), a triangle for yellow spores released at \(z_{src}/h = 2/3\), and a circle for red spores released at \(z_{src}/h = 1/3\). Rotorod spore collectors were deployed on nine vertical poles (numbered 1–9) at locations indicated by crosses to measure mean concentration, while slides were placed at locations indicated by squares to measure mean ground deposition rate.

row and the source location form a straight line parallel to the row of maize, and parallel side rows are 0.76 m away from the centre row. The three columns of poles placed 2 m \((X/h \approx 1)\), 4 m \((X/h \approx 2)\), and 8 m \((X/h \approx 4)\) downwind from the source (hereafter \((x,y)\) are used as coordinates along the mean wind direction and \((X,Y)\) along the experimental grid). During the release experiment studied here, the angle \(\phi\) formed between the steady mean wind at the canopy top and the centre line of the sampling array was \(-2.4\) degrees, with a standard deviation of 30 degrees. Rotorods were placed on each pole at the same five heights as those of sonic anemometers to collect spores, forming a three-dimensional sampling array containing 45 samplers (crosses in Fig. 3.3).

Fig. 3.4 compares LES results and field experimental data for normalized mean concentration \((\overline{C}/Q)\). The majority of LES predictions are within a factor of two of observations, an improvement over the results of the gradient-diffusion model used by Skelsey et al. (2008) [46] which gave predictions within a factor of ten of observations. Quantitative measurements of model performance are provided
in Table 3.2 using three metrics commonly used in the evaluation of dispersion models [113]: the geometric mean bias

\[
MG = \exp \left[ \frac{1}{N} \sum_{i=1}^{N} \left( \ln (\frac{C_i/Q}{Q_{obs}}) - \ln (\frac{C_i/Q}{Q_{LES}}) \right) \right],
\]

the geometric variance

\[
VG = \exp \left[ \frac{1}{N} \sum_{i=1}^{N} \left( \ln (\frac{C_i/Q}{Q_{obs}}) - \ln (\frac{C_i/Q}{Q_{LES}}) \right)^2 \right],
\]

and the fraction of predictions within a factor of two of observations

\[
FAC2 = \text{fraction of data that satisfy } 0.5 \leq \frac{(C/Q)_{obs}}{(C/Q)_{LES}} \leq 2.0.
\]

Here \(N\) is the sample size while subscripts “LES” and “obs” indicate simulation results and observations, respectively. A perfect dispersion model corresponds to \(MG = 1\), \(VG = 1\), and \(FAC2 = 100\%\). Chang and Hanna (2004) suggest that a dispersion model should be considered good if the mean bias is within ±30\% of the mean (0.7 < MG < 1.3), the random scatter is within a factor of two of the mean (VG < 1.6), and \(FAC2 > 50\%\) [9]. Table 3.2 reveals a monotonic trend of improving results with increasing source height, independent of the models adopted for the drag coefficient. This is seen as a decrease of VG (getting closer to 1) and an increase of \(FAC2\), corresponding to the reduction of scatter in Fig. 3.4. These results reflect the difficulty of modeling sources deep inside the canopy, where the dispersion of particles carried by isolated events and small eddies as well as the deposition onto canopy elements and the ground play a critical role. Table 3.2 also shows that LES using \(C_d = (|\tilde{u}|/A)^B\) provides the most accurate results, meeting the standard of a good dispersion model suggested by Chang and Hanna (2004) [9] (except for VG of particles released at \(z_{src}/h = 1/3\)). The performance of LES employing \(C_d = \text{constant}\) is inferior to that of LES using \(C_d = (|\tilde{u}|/A)^B\), most notably for particles released at \(z_{src}/h = 1\) and \(1/3\). For particles released at \(z_{src}/h = 2/3\), the model used for \(C_d\) affects the profiles of mean concentration at individual locations (shown in Fig. 3.5 and discussed below), but induces negligible changes in the overall statistics (Table 3.2). The consistent bias in the comparisons between model and observations for \(z_{src}/h = 2/3\) may be due to an underestimation of the source strength from the experimental run. Results obtained by using an
Figure 3.4. Comparison of LES results and field experimental data for normalized mean concentration \(\overline{C}/Q\) shown using pentagrams for spores released at \(z_{\text{src}}/h = 1\) (a, d), triangles for spores released at \(z_{\text{src}}/h = 2/3\) (b, e), and circles for spores released at \(z_{\text{src}}/h = 1/3\) (c, f). Subscripts “LES” and “obs” indicate LES predictions and field observations, respectively. Simulations were conducted using \(C_d = \text{constant}\) (a–c) and \(C_d = (|\tilde{u}|/A)^B\) (d–f). Solid lines indicate the 1:1 line, and dash lines indicate a scatter of a factor of two.

LSM ([4], in which turbulence statistics were calculated using a second-order closure model) are also shown in Table 3.2, illustrating the superior performance of the LES model.

Fig. 3.5 compares LES results and field experimental data for the profiles of mean concentration \(\overline{C}/Q\). As noted above, the inclusion of plant reconfiguration improves the agreement between model and observations for spores released at \(z_{\text{src}}/h = 1\) (black solid lines compared with dash lines evaluated against pentagrams in Fig. 3.5), and most of the improvement occurs inside the canopy at near poles (poles 1–6, \(X/h \leq 2\)). This result is consistent with the underestimation of sweeps in the simulation using \(C_d = \text{constant}\) (Fig. 3.2d), because strong sweeps transport spores downward in the canopy more quickly than the smaller and less organized eddies. Despite this improvement, a considerable underestimation is still observed inside
the canopy on the lateral poles (mostly on poles 1 and 3). Two possible explanations for this mismatch are the remaining underestimation of sweeps (Fig. 3.2d) and the underestimation of $\sigma_v$ by 20% that can lead to reduced lateral spread of the plume (Fig. 3.1e). The predictions of mean concentration profile at the far poles (poles 7–9, $X/h \approx 4$) are not very sensitive to the model used for $C_d$.

For spores released at $z_{src}/h = 2/3$, concentrations below the source height are also increased by the inclusion of the canopy reconfiguration mechanism (*black solid lines* compared with *dash lines* evaluated against *triangles* in Fig. 3.5). The most noticeable feature of the comparison for this case is the significant improvement in the predictions of mean concentration profile at far poles (poles 7–9) produced by the inclusion of the reconfiguration (*black solid lines* in Fig. 3.5c, f, i). The main feature of the comparison for spores released at $z_{src}/h = 1/3$ is the large overestimation of concentrations close to the ground (*black lines* evaluated against *circles* in Fig. 3.5). This is accompanied by an underestimation above the canopy, suggesting that the LES has difficulties in capturing the vertical transport for sources deep inside the canopy. Once again, inclusion of reconfiguration improves agreement at far poles (poles 7–9).

Fig. 3.6 compares LES results and field experimental data for mean ground

| $z_{src}/h$ | Statistics | $C_d = \text{constant}$ | $C_d = (|\tilde{u}|/A)^B$ | LSM |
|------------|------------|-------------------|-------------------|------|
| 1          | MG         | 1.24              | 1.02              | 1.87 |
|            | VG         | 1.33              | 1.17              | 2.05 |
|            | FAC2       | 88%               | 93%               | 55%  |
| 2/3        | MG         | 0.65              | 0.70              | 1.13 |
|            | VG         | 1.41              | 1.41              | 1.80 |
|            | FAC2       | 74%               | 70%               | 67%  |
| 1/3        | MG         | 0.70              | 1.09              | 1.02 |
|            | VG         | 2.00              | 2.18              | 1.45 |
|            | FAC2       | 61%               | 66%               | 71%  |

Table 3.2. Quantitative evaluation of LES-predicted normalized mean concentration field ($C/Q$) for simulations using $C_d = \text{constant}$ and $C_d = (|\tilde{u}|/A)^B$ against field experimental data using MG, VG, and FAC2. LSM results against the same experimental data are from Gleicher et al. (2014) [4]. A perfect model corresponds to MG = 1, VG = 1, and FAC2 = 100%; Chang and Hanna (2004) suggests $0.7 < \text{MG} < 1.3$, VG < 1.6, and FAC2 > 50% for a good model [9].
Figure 3.5. Comparison of LES results and field experimental data of normalized mean concentration (\(\overline{C}/Q\)) against normalized height (\(z/h\)). See Fig. 3.3 for pole locations. Experimental data are indicated by pentagrams, triangles, and circles for spores released at \(z_{src}/h = 1, 2/3,\) and \(1/3\), respectively. Dash and solid lines indicate results given by LES using \(C_d = \text{constant}\) and \(C_d = (|\tilde{u}|/A)^B\), respectively. Black and grey lines indicate results given by LES with canopy deposition model activated and deactivated, respectively.
deposition rate $\Phi_G/Q$, where $\Phi_G = \left[w_s \bar{C} - \bar{wC}\right]_{z=0}$. During the field experiment, deposition was measured along the centerline at distance from the source corresponding to $X/h \approx -1/2, 1/2, 1, 3/2, 2, 5/2, 3, 7/2, \text{and} 4$ (squares in Fig. 3.3). For spores released at $z_{src}/h = 1$, the agreement between LES results and field experimental data of $\Phi_G/Q$ is unsatisfactory, regardless of the treatment of $C_d$ (Fig. 3.6a), even though the model performance of $\bar{C}/Q$ is good (Fig. 3.5). Field experimental data of $\Phi_G/Q$ obtained using a small sampling area ($3.2 \text{ cm}^2$) are less representative than measurements of $\bar{C}/Q$ obtained using a large sampling volume ($0.1 \text{ m}^3$). For spores released at $z_{src}/h = 2/3$ and $1/3$, LES treating $C_d$ as a constant fails to reproduce the trend of $\Phi_G/Q$ against downwind distance $x$ (dash lines in Fig. 3.6b, c). The best model performance is obtained by LES using $C_d = (|\tilde{u}|/A)^B$, even though the agreement is still mediocre. Better prediction of $\Phi_G/Q$, possibly due to better prediction of $\bar{C}/Q$, is obtained for spores released at $z_{src}/h = 2/3$ than for spores released at $z_{src}/h = 1/3$ (black solid lines in Fig. 3.6b, c).

In addition to the simulations analyzed in Fig. 3.4, simulations using $C_d = (|\tilde{u}|/A)^B$ were conducted without deposition on canopy elements for particles released at each of the three source heights. For all source heights, disregarding deposition on canopy elements induces differences in mean concentration profiles and mean ground deposition rate, which become increasingly apparent with downwind distance $x$ (grey solid lines compared with black solid lines in Fig. 3.5 and 3.6). As expected, deposition on canopy elements induces small changes of $\bar{C}/Q$ at near
poles (poles 1–6, \(X/h \leq 2\)). These results suggest that \(x/h \gtrsim 4\) is an appropriate distance for evaluation of canopy deposition models for light particles.

### 3.4 Characterization of Particle Plume

The canopy-resolving LES model including plant reconfiguration parameterized through \(C_d = (|\tilde{u}|/A)^B\) provides the best reproduction of turbulence statistics, mean concentration, and mean ground deposition rate. Consequently, results from this model are used for the analysis in this section. Here the focus is on vertical dispersion of particles released inside the canopy. Thus, the mean concentration field is integrated in crosswind direction over the simulation domain width, i.e., \(\chi(x, z) = \int_y \overline{C} dy\). In Section 3.4.1 mass balances are used to obtain estimates of the escape fraction (EF), an essential parameter in quantifying plume strength above the canopy. Geometric characteristics of the spatial distribution of crosswind-integrated normalized mean concentration \((\chi(x, z)/Q)\) are studied in Section 3.4.2.

#### 3.4.1 Mass Balances and Escape Fraction

The mass balances are investigated based on the conservation equation for mean concentration \(\overline{C}\) in steady state,

\[
\frac{\partial \overline{C}}{\partial t} = 0 = Q\delta(x)\delta(y)\delta(z-z_{src}) - \left[ \frac{\partial}{\partial x} \overline{uC} + \frac{\partial}{\partial y} \overline{vC} + \frac{\partial}{\partial z} \overline{wC} - w_s \frac{\partial \overline{C}}{\partial z} \right] - S_p + D \nabla^2 \overline{C},
\]

where \(Q\) is the rate of release from a point source located at \((x, y, z) = (0, 0, z_{src})\), \(\delta\) is the Dirac delta function, \(S_p\) is the rate of deposition on canopy elements, and \(D \nabla^2 \overline{C}\) is the rate of Brownian diffusion (neglected hereafter). Integrating Eq. (3.7) in the crosswind direction from \(y \rightarrow -\infty\) to \(y \rightarrow \infty\) (also denoted as \(\int_y\)) yields

\[
0 = Q\delta(x)\delta(z-z_{src}) - \frac{\partial}{\partial x} \int_y \overline{uC} dy - \frac{\partial}{\partial z} \int_y \overline{wC} dy + w_s \frac{\partial}{\partial z} \int_y \overline{C} dy - \int_y S_p dy. \tag{3.8}
\]

The global mass balance is obtained by integrating Eq. (3.8) in vertical direction from \(z = 0\) to \(z \rightarrow \infty\) and then in downwind direction from \(x \rightarrow -\infty\) to some
arbitrary downstream distance $x > 0$ (hereafter denoted as $f_x$),

$$0 = Q - \int_{z=0}^{z=\infty} \int_y \overline{uC} dydz - \int_x \int_y \Phi_G dydx - \int_x \int_{z=0}^{z=h} \int_y S_p dydzdx. \quad (3.9)$$

Here $\Phi_G = [\overline{w_sC} - \overline{wC}]_{z=0}$ is the mean ground deposition rate. Eq. (3.9) implies that particles released from the point source ($Q$) are either transported downwind (the term associated with $\overline{uC}$) or removed by deposition on the ground (the term associated with $\Phi_G$) and canopy elements (the term associated with $S_p$). The fraction of particles remaining airborne ($AF$) has to be identical to the rate of particles transported downwind ($F_T/Q$),

$$AF \equiv 1 - f_{\Phi_G} - f_{S_p} = \frac{F_T}{Q} = \frac{\int_{z=0}^{z=\infty} \int_y \overline{uC} dydz}{Q},$$

where the fraction removed by deposition on ground is

$$f_{\Phi_G} = \frac{\int_x \int_y \Phi_G dydx}{Q}, \quad (3.11)$$

and the fraction removed by deposition on canopy elements is

$$f_{S_p} = \int_x \int_{z=0}^{z=h} \int_y S_p dydzdx/Q. \quad (3.12)$$

As expected, this global mass balance is satisfied by all LES case studies. Examples for particles released at $z_{src}/h = 1, 2/3$, and $1/3$ are shown in Fig. 3.7 (black plus signs compared with black solid lines). Heavy particles released deep inside the canopy are completely depleted within a short distance downwind from the source. As an example, in Fig. 3.7(f) $AF \approx 0$ at $x/h \gtrsim 2$.

Particles with negligible gravitational settling velocity ($w_s/u_* \ll 1$) that escape the canopy mostly remain above the canopy, while those particles that do not escape are depleted within a few canopy heights downwind of the source. This behavior leads to an equilibrium away from the source so that $AF$ becomes approximately constant, as displayed in Fig. 3.7(e) at $x/h \gtrsim 6$. Particles with non-negligible gravitational settling velocity that escape the canopy close to the source settle back into the canopy, where they are deposited along with those particles that do not escape the canopy. Consequently, for these particles $AF$ away from the source.
gradually decreases with downwind distance \((x)\), as depicted in Fig. 3.7(b, d).

A second mass balance is conducted for the region above the canopy by integrating Eq. (3.8) in vertical direction from \(z = h\) to \(z \to \infty\) and then in downwind direction from \(x \to -\infty\) to some arbitrary downstream distance \(x > 0\), resulting in

\[
\int_{z=h}^{z\to\infty} \int_y \bar{u} \bar{C} \, dy \, dz = \int_x \int_y \left[ \bar{w} \bar{C} - w_s \bar{C} \right]_{z=h} \, dy \, dx,
\]

where \(\left[ \bar{w} \bar{C} - w_s \bar{C} \right]_{z=h}\) is the flux of particles out of the canopy layer. Thus the fraction of particles escaping the canopy layer (EF) should be identical to the flux of particles transported downwind above the canopy \((F_{T,z>h}/Q)\),

\[
EF = \frac{\int_x \int_y \left[ \bar{w} \bar{C} - w_s \bar{C} \right]_{z=h} \, dy \, dx}{Q} = \frac{\int_x \int_y \bar{u} \bar{C} \, dy \, dz}{Q} = \frac{F_{T,z>h}}{Q}.
\]  (3.14)

This requirement is satisfied by most LES runs, except for those with particles released at \(z_{src}/h = 1\) (grey plus signs compared with grey solid lines in Fig. 3.7). The discrepancy can be tracked to the interpolations required in the postprocessing stage. The LES model computes \(\bar{u}\) and \(\bar{C}\) on the same grid and \(\bar{w}\) on a staggered grid, so that the calculation of vertical turbulent transport at a given vertical grid \(k\) involves interpolation of the resolved concentration,

\[
\bar{w}'C'_{LES,k} = \bar{w}_k \left( \frac{\bar{C}_k + \bar{C}_{k-1}}{2} \right) + \bar{C}_z^{\bar{C}}.
\]  (3.15)

This approximation is inaccurate close to the source, and therefore runs with particles released at \(z_{src}/h = 1\) fail to satisfy Eq. (3.14). As a result, the most reliable estimate of EF from LES results is \(EF = F_{T,z>h}/Q\), which is used hereafter. In each simulation, EF increases with \(x\) near the source and then it starts decreasing farther away (grey solid lines in Fig. 3.7). This transition trends towards the source as gravitational settling increases in importance. For example, it occurs at \(x/h \approx 6\) for particles having \(w_s/u_* \approx 0.04\) (Fig. 3.7a, c, e) and \(x/h \approx 2\) for particles having \(w_s/u_* \approx 0.2\) (Fig. 3.7b, d). The maximum value of EF is determined by the dispersion process before the transition point. Increasing \(w_s/u_*\) decreases the maximum value of EF and makes the decrease of EF greater after the maximum is reached. For a fixed value of \(w_s/u_*\), EF increases with \(z_{src}/h\). The portion of released particles that remain inside the canopy, represented by the difference
Figure 3.7. LES results against normalized downwind distance \((x/h)\) for fractions of particles transported downwind \((F_T/Q; \text{black solid lines})\), removed by deposition on the ground \((F_{\Phi_G}; \text{black dash lines})\), removed by deposition on canopy elements \((F_{S_p}; \text{black dash-dot lines})\), remaining airborne \((AF; \text{black plus signs})\), transported downwind above the canopy \((F_{T,z>h}/Q; \text{grey solid lines})\), transported downwind by mean flow above the canopy \((F_{T,u,z>h}/Q; \text{grey dash-dot lines})\), and escaping the canopy \((EF; \text{grey plus signs})\), for particles released at \(z_{src}/h = 1\) \((a, b)\), \(2/3\) \((c, d)\), and \(1/3\) \((e, f)\). Simulations were conducted using \(w_s/u_* \approx 0.04\) \((a, e)\) and \(w_s/u_* \approx 0.2\) \((b, d, f)\).
between EF and AF, decreases with downwind distance due to deposition, so that EF approaches AF away from the source (grey solid lines compared with black plus signs in Fig. 3.7).

It is interesting to note that field experimental studies usually assume negligible turbulent contribution to streamwise transport, i.e., \( \overline{u'c'}/\overline{uc} \ll 1 \) and therefore \( \overline{uc} \approx \pi \overline{C} \) [43,143]. These studies estimated escape fraction as \( F_{T,z>h}/Q \), where

\[
F_{T,z>h} = \int_{z=\text{h}}^{z=\infty} \int_{y} \overline{\pi C} dydz. \tag{3.16}
\]

This is usually done near the source \((x/h \leq 2)\), where concentrations are large enough for measurements of \( \overline{C} \) to be accurate. LES results show that the contribution of \( \overline{u'c'} \) is not negligible and such approximation near the source region can introduce an error larger than 20% (grey dash-dot lines compared with grey solid lines in Fig. 3.7).

For each simulation a single value of escape fraction was estimated as the maximum value of \( F_{T,z>h}/Q \) (note that most of the net transport across the canopy top occurs within \( x/h \leq 2 \)). Resulting values of EF are shown as a function of \( z_{\text{src}}/h \) in Fig. 3.8(a). Three regimes can be identified in Fig. 3.8(a), which can be associated with the importance of gravitational settling with respect to vertical turbulence fluctuations \((w_s/\sigma_w)\) shown in Fig. 3.8(b). The first regime, in which gravitational settling dominates over vertical turbulent transport \((w_s/\sigma_w \gtrsim 0.7)\), corresponds to nearly zero escape fraction. This is observed for particles having \( w_s/u_* \approx 0.2 \) released at \( z_{\text{src}}/h \lesssim 1/2 \). The second regime corresponds to the situation where gravitational settling and vertical turbulent transport are comparable \((0.05 \lesssim w_s/\sigma_w \lesssim 0.7)\), so that EF increases as \( w_s/\sigma_w \) decreases. For a fixed value of \( w_s/u_* \), the EF increases with \( z_{\text{src}}/h \) approximately linearly at a constant rate that is independent of \( w_s/u_* \). For a fixed value of \( z_{\text{src}}/h \), the increase of EF due to the decrease of \( w_s/u_* \) is greatest at \( 1/2 < z_{\text{src}}/h < 3/4 \) and then decreases with increasing \( z_{\text{src}}/h \) as the difference in \( w_s/\sigma_w \) decreases. The third regime corresponds to the situation where vertical turbulent transport dominates gravitational settling \((w_s/\sigma_w \lesssim 0.05)\), so that EF becomes approximately a constant. This is observed for particles having \( w_s/u_* \approx 0.04 \) released in the upper 20% of the canopy. Syntheses of these findings suggest two regimes with approximately constant escape fraction (zero in the deep canopy where \( w_s/\sigma_w \gtrsim 0.7 \) and a maximum value near the canopy.
Figure 3.8. LES results of escape fraction (EF) estimated as the maximum of $F_{T,z > h}/Q$ against normalized source height ($z_{src}/h$) (a) and the relative importance of gravitational settling and vertical turbulence transport ($w_s/u_*$) against normalized height ($z/h$) (b). Solid lines with circles and squares indicate results given by LES conducted using $w_s/u_* \approx 0.04$ and $w_s/u_* \approx 0.2$, respectively.

top where $w_s/\sigma_w \lesssim 0.05$) with an approximately linear transition in between characterized by constant and perhaps universal slope.

3.4.2 Plume Model

Fig. 3.9 shows the spatial distribution of normalized mean concentration integrated in crosswind direction ($\chi(x,z)/Q$) for selected simulations, illustrating the effects of $z_{src}/h$ and $w_s/u_*$. For simulations in which $w_s/\sigma_w \gtrsim 0.7$ at the source height, as illustrated in Fig. 3.9(f), the plume is confined to the region inside the canopy. This result is consistent with the near-zero escape fraction (EF) displayed in Fig. 3.8(a). Within about two canopy heights downwind from the source, most of the plume is depleted by deposition onto canopy elements and the ground. Note the remarkable difference between the plumes shown in Fig. 3.9(d, f). In the case shown in Fig. 3.9(f), ground deposition is slightly larger than canopy deposition (see Fig. 3.7f). All simulations with $w_s/u_* \approx 0.2$ and $z_{src}/h \lesssim 1/2$ present similar behaviour, in that the plumes are highly confined to very short distances downwind of the source within the canopy region. Consequently, these cases are not included in the analysis of the mean plume presented in this section.

The growth of the mean concentration plume can be characterized by its centroid
Figure 3.9. LES results depicting iso-contours of mean concentration integrated in crosswind direction ($\chi$) normalized by point source strength ($Q$) plotted in $x/h$ (downwind) and $z/h$ (vertical) space for particles released at $z_{src}/h = 1$ (a, b), $2/3$ (c, d), and $1/3$ (e, f). Simulations were conducted using $w_s/u_* \approx 0.04$ (a, c, e) and $w_s/u_* \approx 0.2$ (b, d, f). Pentagrams, triangles, and circles indicate point sources located at $z_{src}/h = 1$, $2/3$, and $1/3$, respectively. Dots, dash lines, and plus signs indicate LES results for $\bar{z}/h$, $(\bar{z} \pm \sigma_z)/h$, and the location of the maximum of $\chi(x, z)$ at a given $x$, respectively. Solid lines indicate $\bar{z}/h = 0.68(x/h)^{0.35}$ in panels (a), (e), and (e) and $\bar{z}/h = 0.8(x/h)^{0.3}$ in panels (b) and (d).
defined as the mean vertical displacement

\[ \tau(x) = \frac{\int_{z=0}^{z=\infty} z \chi(x, z) dz}{\int_{z=0}^{z=\infty} \chi(x, z) dz}, \]  

(3.17)

and a mean vertical length scale of the plume defined as the standard deviation of vertical displacement

\[ \sigma_z(x) = \left( \frac{\int_{z=0}^{z=\infty} (z - \tau)^2 \chi(x, z) dz}{\int_{z=0}^{z=\infty} \chi(x, z) dz} \right)^{1/2} = (\bar{z}^2 - \tau^2)^{1/2}. \]  

(3.18)

These quantities are displayed in Fig. 3.9(a–e), where the vertical location of the peak concentration \( z_{\text{max}} \) is also shown as a function of \( x \). For sources near the canopy top, \( z_{\text{max}} \) is constant and coincides with \( h \) (Fig. 3.9a, b). For sources deeper inside the canopy, the behaviour of \( z_{\text{max}} \) can be separated into three regions. In the first region, \( z_{\text{max}} \) moves towards the ground. In this region \( \tau \) decreases with \( x \) (at a rate controlled by \( w_s/u_* \)) and the growth of \( \sigma_z(x) \) is dictated by the local values of \( \sigma_w \) (i.e., it is slower for particles released deep inside the canopy, where \( \sigma_w/u_* \) is smaller, than for those released close to the canopy top). These patterns are clearly demonstrated in Fig. 3.10 for all simulations of interest. In the second regime, \( z_{\text{max}} \) stays at the ground. The growth rates of \( \tau \) and \( \sigma_z \) increase with \( x \) due to depletion of particles inside the canopy caused by deposition on the ground and canopy elements. The continuous depletion leads to a sudden change of \( z_{\text{max}} \) from ground (\( z = 0 \)) to canopy height (\( z = h \)). The transition takes place closer to the source in simulations using greater \( w_s/u_* \), due to rapid depletion, than those using smaller \( w_s/u_* \). It also occurs farther downwind for those with lower \( z_{\text{src}}/h \), due to the large amount of particles inside the canopy to be depleted, than those using higher \( z_{\text{src}}/h \). For cases simulated here, all transitions occur within \( x/h < 8 \).

The most important point, however, is that both \( \tau(x) \) and \( \sigma_z(x) \) display a power-law dependence on downwind distance \( x \) once the transition to \( z_{\text{max}}/h = 1 \) is reached (this being the third region). If representations \( \tau(x) \propto x^{\gamma_1} \) and \( \sigma_z(x) \propto x^{\gamma_2} \) are adopted, then the parameters \( \gamma \) are independent of \( z_{\text{src}}/h \) (our empirical fits suggest \( \gamma_1 = 0.35 \) and \( \gamma_2 = 0.40 \) for \( w_s/u_* \approx 0.04 \) and \( \gamma_1 = 0.30 \) and \( \gamma_2 = 0.40 \) for \( w_s/u_* \approx 0.2 \)). In this third region \( \tau(x) \) and \( \sigma_z(x) \) essentially collapse to a common curve for particles released at different \( z_{\text{src}}/h \) (Fig. 3.10). The collapse of LES results of \( \sigma_z/h \) was also observed by Prabha et al. (2008) for passive scalars released
from point sources at different heights inside a plant canopy [68]. The values of $\gamma$ estimated from the LES are also consistent with laboratory data showing $\gamma_2 = 0.35$ for passive scalars released at $z_{src}/h = 0.85$ in a model canopy [144]. As it will be shown below, a different coordinate system is more appropriate to analyze these power-law regimes.

These results encourage the development of simple analytical models for the plume dispersal above the canopy. Our goal is to obtain a simple model valid above the canopy in which a virtual source is used to reproduce the concentration field from the real source but to avoid the intractable task of modeling dispersion inside the canopy. Despite the results of $\overline{u'c'}/\overline{uc}$ from Section 3.4.1, obtaining analytical solutions requires the assumption that turbulent transport in the streamwise direction be negligible in comparison to mean advection (i.e., $\overline{uc} = \overline{\pi c} + \overline{w\sigma z} \approx \overline{\pi(z)c}$). Invoking an eddy-diffusivity closure to the turbulent transport in the vertical direction (i.e., $\overline{w\sigma z} = -K_z(z)(\partial \overline{c}/\partial z)$) and neglecting gravitational settling allow one to rewrite Eq. (3.8) as

$$0 = -\overline{\pi(z)} \frac{\partial \chi}{\partial x} + \frac{\partial}{\partial z} \left( K_z(z) \frac{\partial \chi}{\partial z} \right).$$

The small effect on $\overline{z}(x)$ and $\sigma_z(x)$ resulting from the five fold increase in $w_s/u_*$ revealed in Fig. 3.10 suggests that the effects of gravitational settling on plume
growth above the canopy are not large. This is in part due to the small values of $w_s/\sigma_w$ observed at the canopy top (see Fig. 3.8b).

In order to obtain analytical solutions to Eq. (3.19), power-laws are assumed for mean velocity and vertical eddy-diffusivity profiles [145]

$$\bar{w}(z) = C_p u_* \left( \frac{z - d}{z_0} \right)^m,$$

$$K_z(z) = \kappa u_* l \left( \frac{z - d}{z_0} \right)^n.\tag{3.21}$$

Here, $\kappa = 0.4$ is the von Kármán constant, $z_0$ and $d_0$ are the roughness length scale and the displacement height, $l$ is an additional length scale, and $C_p$, $m$, and $n$ are dimensionless constants. All these parameters and constants have well defined values in the surface layer [92], but here the focus is on the canopy roughness sublayer where the values need not to be the same. Therefore, values are obtained from fitting the profiles to LES output, shown in Fig. 3.11(a, b). The empirical fits are performed in the region $4/3 < z/h < 7/2$, where the normalized mean-square error (NMSE) of fitting $K_z = -\bar{w}'C'/(\partial C/\partial z)$ is below 0.1 (Fig. 3.11c). This region ($4/3 < z/h < 7/2$) is also where the majority of the plume is located (Fig. 3.9). At each vertical level $k$, the NMSE measures the difference between LES results and fitted mean vertical turbulent fluxes,

$$\text{NMSE}_k = \frac{\Sigma \left( w' C'_{\text{Fit},k} - w' C'_{\text{LES},k} \right)^2}{\Sigma \left( w' C'_{\text{LES},k} \right)^2}.\tag{3.22}$$

Here, $w' C'_{\text{LES},k}$ is calculated using Eq. (3.15) and

$$w' C'_{\text{Fit},k} = -K_{z,k} \frac{\bar{C}_k - \bar{C}_{k-1}}{\Delta z}.\tag{3.23}$$

Fits of eddy-diffusivity are performed using data for $x/h \gtrsim 2$ from simulations using $w_s/u_* \approx 0.04$ and for $x/h \gtrsim 1$ from simulations using $w_s/u_* \approx 0.2$ (this is done to eliminate the region close to the source). Based on the fits we use $z_0/h \approx 1/8$, $d/h \approx 7/8$, and $l/h \approx 0.46$ and dimensionless constants $C_p \approx 2.88$, $m \approx 0.39$, and $n \approx 0.38$. Fig. 3.11 shows that the power-law assumptions yield satisfactory fits to the mean velocity and eddy-diffusivity profiles. The NMSE associated with eddy
Figure 3.11. Normalized mean velocity ($\bar{u}/u_*$; a), eddy-diffusivity ($K_z$; b), and the normalized mean-square error (NMSE) of fitted $K_z$ (c) against normalized height ($z/h$). Black dots indicate LES results, while grey solid lines indicate fitting of Eq. (3.20) and (3.21) at $4/3 < z/h < 7/2$, the region where the NMSE of fitted $K_z$ is less than 0.1.

diffusivity estimated inside the canopy is very large (Fig. 3.11c), consistent with the notion that eddy-diffusivity models are not very accurate inside plant canopies.

Downstream from the location where $z_{\text{max}}/h = 1$ is reached, $z_{\text{max}}$ stays at the canopy top, suggesting that the virtual origin of the plume should also be located at $z = z_{\text{max}} \approx h$. However, to obtain an analytical solution for Eqs. (3.19)–(3.21), the virtual origin must coincide with the height where the mean velocity and eddy diffusivity vanish ($z = d$). This approximation is acceptable, because $d \approx h$. As a result, (3.19) is solved for the case of a virtual continuous point source with strength $Q_v$ located at $(x,z) = (x_0,d)$ and a domain $(x \geq x_0, z \geq d)$. The boundary conditions are

$$\chi \to \infty \text{ at } x = x_0, \ z = d, \quad (3.24)$$

$$\chi \to 0 \text{ as } x, z \to \infty. \quad (3.25)$$

In addition, it is assumed that the maximum of $\chi(x,z)$ at any given $x > x_0$ is located at $z = d$, implying

$$\frac{\partial \chi}{\partial z} \to 0 \text{ as } z \to d, x > x_0. \quad (3.26)$$

Eq. (3.26) is equivalent to assuming no mean vertical concentration flux at $z = d$. Therefore, this boundary condition does not allow particles to penetrate into the
canopy region. Note that the effects of settling velocity are expected to be small, given the small values of \( \frac{w_s}{\sigma_w} \) above the canopy. However, the mean drift of particles into the canopy due to gravitational settling is expected to introduce differences between the theoretical model and LES results for heavier particles.

The analytical solution to the problem described above is given by

\[
\frac{\chi(x, \zeta)}{Q_v} = \frac{r z_0^m}{C_p u_s \Gamma(s)} \left[ \frac{C_p z_0^{n-m}}{r^2 \kappa l (x - x_0)} \right]^s \exp \left[ - \frac{C_p z_0^{n-m} \zeta^r}{r^2 \kappa l (x - x_0)} \right]. \tag{3.27}
\]

This is consistent with the solution first proposed by Sutton (1953) [146] for a similar problem. Here, \( \zeta = z - d \), \( r = m - n + 2 > 1 \) and \( s = (m + 1)/r \).

The analytical solution, Eq. (3.27), gives an estimation of the growth of the plume above the canopy characterized by the mean vertical displacement,

\[
\bar{\zeta} = \frac{\Gamma(2/r)}{\Gamma(1/r)} \left( \frac{r^2 \kappa l}{C_p z_0^{n-m}} \right)^{1/r} (x - x_0)^{1/r}, \tag{3.28}
\]

and the standard deviation of vertical displacement,

\[
\sigma_\zeta = \frac{[\Gamma(3/r) \Gamma(1/r) - \Gamma(2/r) \Gamma(2/r)]^{1/2}}{\Gamma(1/r)} \left( \frac{r^2 \kappa l}{C_p z_0^{n-m}} \right)^{1/r} (x - x_0)^{1/r}. \tag{3.29}
\]

Here, \( \bar{\zeta} \) and \( \sigma_\zeta \) are defined similarly to \( \bar{\sigma} \) and \( \sigma_\sigma \) by replacing \( \bar{z} \) with \( \zeta \) in Eqs. (3.17) and (3.18). Several interesting features are revealed by these equations. Firstly, the growth rates of \( \bar{\zeta} \) and \( \sigma_\zeta \) are the same, given by \( (x - x_0)^{1/r} \). Secondly, \( 1/r \) is determined by the power-law exponents of the mean velocity and eddy-diffusivity profiles. The increase in eddy-diffusivity with height enhances \( 1/r \), while the increasing mean velocity reduces \( 1/r \). In the canopy roughness sublayer, fits to the LES profiles yield \( m \approx 0.39 \), and \( n \approx 0.38 \), so that the two effects cancel out and the analytical model yields \( 1/r \approx 0.5 \) (the same growth rate expected in homogeneous isotropic turbulence [60], but for a different reason). Typically in the neutral surface layer (i.e., the log-layer) \( m = 1/7 \) and \( n = 6/7 \) [145], so that \( 1/r \approx 7/9 \) and the plume grows much faster than in the canopy roughness sublayer.

Predictions from the analytical model are compared with LES results in Fig. 3.12. Substituting the constants fitted from LES simulations into Eqs. (3.28) and (3.29) results in \( \bar{\zeta}/h \approx 0.41(x/h)^{0.5} \) and \( \sigma_\zeta/h \approx 0.31(x/h)^{0.5} \), with a constant ratio
between the two given by $\zeta/\sigma \approx 1.32$. As a comparison, fits to LES results yield $\zeta/h \approx 0.33(x/h)^{0.5}$, $\sigma_{\zeta}/h \approx 0.24(x/h)^{0.5}$, and $\zeta/\sigma_{\zeta} \approx 1.38$. The overestimation of the growth of $\zeta$ and $\sigma_{\zeta}$ given by Eqs. (3.28) and (3.29) (see Fig. 3.12a, b) are most likely caused by the approximation made to the lower boundary conditions Eqs. (3.24) and (3.26). Inspection of Fig. 3.12(c, d) reveals that most of the overprediction in Eqs. (3.28) and (3.29) originates from the early-stage growth of the plume (the region $x/h \leq 4$), supporting this explanation.

The boundary condition, Eq. (3.26), implies that all the particles emitted by the virtual source will remain above the canopy. Consequently, a logical choice for the strength of the virtual source is $Q_v = Q \cdot EF$, where $EF$ is the maximum escape fraction shown in Fig. 3.8. Note that this is equivalent to assuming $F_{T,z>h} \approx$
constant, which is not exactly true (due primarily to gravitational settling, as discussed earlier). Therefore, some deviations between theoretical model predictions and LES results are expected.

The mean plume produced by the theoretical model (Fig. 3.13a) is compared with LES results for light and heavy particles released at $z_{src}/h = 2/3$ (Fig. 3.13b, c). In these panels, $EF$ is estimated as the maximum of $F_{T,z>h}/Q$ and $x_0 \approx 0$ is used and gives a good approximation. The agreement for light particles is good, except in the upper part of the plume ($z/h > 3$) where concentrations are small ($\chi/(Q \cdot EF) < 0.01 \text{ s m}^{-2}$; see Fig. 3.13a, b). Particles having $w_s/u_* \approx 0.2$ show non-negligible rate of decrease of $EF$ with $x$ beyond its maximum location (Fig. 3.7b, d), leading to an increase in the difference between theoretical predictions and LES results for $\chi/(Q \cdot EF)$ (Fig. 3.13a, c). To verify that this difference is primarily due to gravitational settling of particles back into the canopy regions, we show in Fig. 3.13(d) the LES results using $EF$ as the local $F_{T,z>h}/Q$ instead of the maximum of $F_{T,z>h}/Q$. The improvement in agreement between theoretical predictions and LES results for $\chi/(Q \cdot EF)$ is clear (Fig. 3.13a, d).

A quantitative comparison between theoretical predictions and LES results is presented in Fig. 3.14, where profiles of $\chi(x,z)/(Q \cdot EF)$ at selected downwind distances are shown. For particles having $w_s/u_* \approx 0.04$, there is little discernible difference throughout the entire simulation domain between the results from the two approaches to estimate $EF$ (black solid and dash lines collapse in Fig. 3.14a, c, e). For particles having $w_s/u_* \approx 0.2$, values of $\chi(x,z)/(Q \cdot EF)$ given by estimating $EF$ as the local $F_{T,z>h}/Q$ are greater than those given by estimating $EF$ as the maximum of $F_{T,z>h}/Q$. This difference becomes increasingly evident at $x/h \gtrsim 5$ (black dash lines compared with black solid lines in Fig. 3.14d, f). The values of $\chi(x,z)/(Q \cdot EF)$ using $EF$ as the local $F_{T,z>h}/Q$ agree better with theoretical prediction in the region away from the source (e.g., at $x/h \approx 18$) than values using $EF$ as the maximum of $F_{T,z>h}/Q$ (black dash lines compared with black solid lines evaluated against grey lines in Fig. 3.14f). Note that good agreement between LES results and theoretical predictions is observed at $x/h \gtrsim 2$ (Fig. 3.14a, b), even though in many cases the assumptions for Eq. (3.27) are valid only in the region away from the source, e.g., at $x/h \gtrsim 6$ and at $x/h \gtrsim 8$ for particles having $w_s/u_* \approx 0.04$ released at $z_{src}/h = 2/3$ (Fig. 3.9c) and 1/3 (Fig. 3.9e), respectively.
3.5 Conclusions

This work demonstrates the capability of LES models in reproducing the turbulence statistics and mean concentration field resulting from three-dimensional dispersion of particles inside the plant canopy roughness sublayer. The poor performance of LES models in predicting the skewness of the velocity profiles presented in most comparisons between LES results and field observations [53–57] has been tracked to the assumption of a constant drag coefficient in the parameterization.
Figure 3.14. Comparison of theoretical prediction (grey lines) and LES results (black lines) for normalized mean concentration integrated in crosswind direction ($\chi/(Q \cdot EF)$) against normalized height ($z/h$) at normalized downwind distances $x/h \approx 2$ (a, b), 5 (c, d), and 18 (e, f) for particles having $w_s/u_* \approx 0.04$ released at $1/4 < z_{src}/h < 1$ (a, c, e) and having $w_s/u_* \approx 0.2$ released at $1/2 < z_{src}/h < 1$ (b, d, f). Black solid and dash lines indicate LES results using EF estimated as the maximum of $F_{T,z>h}/Q$ and as the local $F_{T,z>h}/Q$ after the maximum is reached, respectively.
of the effects of canopy on the flow field. Plant reconfiguration leads to a drag reduction during strong gusts. This effect was incorporated into the LES by assuming a power-law dependence of the drag coefficient on the velocity. This new formulation for the drag coefficient produces vertical profiles of skewness in good agreement with observations. Furthermore, even though the constant drag coefficient produces an accurate prediction of the mean momentum flux $\overline{u'w'}$, the dynamics of momentum transport into the canopy are incorrect. This is evident from the pronounced underestimation of the fractions of momentum transported by sweeps and strong events (as evidenced by the quadrant-hole analysis). The corresponding underestimation is reduced from 40% to 5% once the reconfiguration mechanism is included. This result suggests that reconfiguration of plants plays an important role in shaping the coherent structures that develop in airflow through maize canopies. It is likely that the importance of reconfiguration mechanism will vary among canopies, depending on the physical characteristics of the plants and their spatial arrangement.

The LES results for particle dispersion are also in good agreement with the measurements for an artificial point-release of Lycopodium spores obtained in the middle of a large cornfield in Mahomet, Illinois on 10 July 2011 [4]. The majority of LES predictions of mean spore concentration are within a factor of two of observations. Results of LES reproduce observations much better than the gradient-diffusion model of Skelsey et al. (2008) [46] and the LSM approach of Gleicher et al. (2014) [4]. To our knowledge, this is the first detailed assessment of LES predictions of particle dispersion within plant canopies that is able to accurately reproduce the three-dimensional mean particle concentration field. The LES approach used here requires only a few input parameters: height-dependent leaf area density, velocity-dependent drag coefficient, friction velocity, settling velocity, and critical velocity for rebound and re-entrainment (used in the canopy deposition model described in Appendix A).

The estimates of escape fraction presented here cannot be assessed against experimental data (no reliable experimental data are available). However, the predictions that no particles escape for large values of $w_s/u_*$ and sources near the ground is in agreement with empirical observation that plant diseases initiated in foci deep within a canopy move upward to the canopy top before spreading across the field and surrounding landscapes.
The mean and standard deviation of vertical displacement of particles show $z_{src}$-independent power-law growth with downwind distance ($x$) once the majority of the plume is above the canopy (marked by the location where the maximum of mean particle concentration integrated in crosswind direction $\chi(x,z)$ at the given $x$ reaches canopy top). This result suggests that away from the source the only relevant effect of source height is captured by the escape fraction. We propose a simple modeling approach in which a virtual source is placed near the top of the canopy. The theoretical solution obtained by Sutton (1953) [146] is applicable to this modified problem and the predictions are in good agreement with LES results for light particles ($w_s/u_* \approx 0.04 \ll 1$). For heavier particles (here represented by $w_s/u_* \approx 0.2$), the agreement is not as good. The discrepancy is traced to the assumption that particles do not settle back into the canopy, and can be corrected if this effect is incorporated into the solution. The theoretical model combines the effects of a variable eddy diffusivity and the mean velocity shear on the mean concentration field. Interestingly, the predictions for the canopy roughness sublayer are very close to the predictions for homogeneous turbulence. However, in the present case, this is due to a compensation between the increase in spread caused by the eddy-diffusivity and a decrease due to the mean shear.

Given the good comparison between theoretical model and LES results, a simple theoretical modeling framework is proposed. The mean concentration field produced by a continuous point source inside the canopy can be represented by two independent sets of parameters: (1) the strength of the plume characterized by the product of the rate of release ($Q$) and the escape fraction ($EF$), and (2) the distribution of normalized mean particle concentration integrated in the crosswind direction given by Eq. (3.27). This representation is readily applicable to parameterization of long-distance dispersal models for particles released inside horizontally homogeneous, uniform crop canopies.
Chapter 4  
Strong and Weak, Unsteady Reconfiguration and Its Impact on Turbulence Structure Within Plant Canopies

4.1 Introduction

Both terrestrial and aquatic plants take advantage of elastic reconfiguration (the bending of plant stems, branches, leaves, and flowers) to reduce drag forces and avoid uprooting or breaking under high winds and currents [125]. The impact of reconfiguration on drag has been described by a modification to the quadratic drag law, which can be modeled by introducing the Vogel number $B$. Specifically, the drag force $F_D \propto U^{2+B}$, with $U$ a characteristic velocity scale acting on the plant element [125,135]. It is sometimes convenient in modeling to transfer the velocity dependence to the drag coefficient, i.e., we write $F_D \propto C_D U^2$, with $C_D \propto U^B$. In the asymptotic regime of negligible reconfiguration, $B \to 0$, and the quadratic increase of drag with velocity is recovered. In the asymptotic regime of strong reconfiguration, dimensional analysis balancing drag force and the plant’s internal resistance to bending suggests specific values of $B$ [2,137]. For linear elastic bending, $B = -2/3$, if reconfiguration is associated with the loss of one characteristic length, such as the bending of a beam or a rectangular plate along a single axis, and $B = -4/3$, if reconfiguration leads to the loss of two characteristic lengths, such
as the crumpling of a paper or the rolling of a disk into a cone. For many aquatic plants the primary restoring force is buoyancy, rather than rigidity. If buoyancy alone is considered as the restoring force $B = -4/3$; and the inclusion of buoyancy in addition to rigidity as restoring forces delays the asymptotic regime of strong reconfiguration to higher values of fluid velocity [3]. These theoretical models predict drag forces in good agreement with laboratory measurements of fibers in soap films [147], rectangular plates in a wind tunnel [136], and model seagrass blades in water [3]. The range $-2/3 \lesssim B \lesssim 0$ is also in rough agreement with many measured values for natural canopies in which one-dimensional bending is observed [127,135,137]. For example, de Langre et al. (2012) reported $B = -0.52$ to $-0.80$ [137], and Albayrak et al. (2012) reported $B = -0.5$ to $-0.7$ [127]. Harder et al. (2004) observed two regimes of behavior for the giant reed (*Arundo donax* L.) [129]. For wind speeds up to 1 m s$^{-1}$, little bending occurred, and the drag force was approximately quadratic ($B \approx 0$), as expected for an unyielding object. However, for wind speeds above 1.5 m s$^{-1}$, significant bending occurred, and the observed $B = -0.7$ was consistent with the scaling for a reconfigured beam ($B = -2/3$).

Although most previous studies have focused on time-averaged flow conditions and the associated mean reconfiguration [127,137], some studies report instantaneous relationships between velocity and reconfiguration [129,131]. Indeed, the phenomena of *honami* and *monami* (progressive waves of canopy bending) are examples of plants bending in response to the passage of individual turbulent eddies [148,149]. We hypothesize that the reconfiguration of plants at time-scales comparable to individual strong events can preferentially allow downward movements associated with these events to penetrate further into a canopy. Specifically, we propose that the drag coefficient responds to the instantaneous velocity, $\mathbf{u} = (u, v, w)$ (a vector consisting of streamwise, spanwise, and vertical components), such that the characteristic velocity $U = |\mathbf{u}|$ and $C_D \propto U^B$ will be smaller for stronger events (higher $|\mathbf{u}|$). Note $|\mathbf{u}|$ is statistically positively correlated with its streamwise component, $u$, so that in general stronger events have higher $u$. The canopy-drag length-scale, $L_c \propto (C_D a)^{-1}$, describes the penetration of turbulent momentum flux into the canopy [8,150]. Here $a$ is the frontal area per volume. If stronger events (higher $u$) experience a smaller $C_D \propto U^B$, then they can penetrate a greater distance into the canopy before being arrested by drag, compared to weaker events.
This impact of plant flexibility should be evident in the skewness of the streamwise and vertical velocities ($Sk_u$ and $Sk_w$, respectively), which are statistical measures of bias toward larger events.

Many studies within a variety of real and model canopies have observed $Sk_u > 0$ and $Sk_w < 0$, indicating the prevalence of events with strong positive $u$ ($u' > 0$) and strong negative $w$ ($w' < 0$), i.e., sweeps [48,82]. Here $u'$ and $w'$ are the deviations of $u$ and $w$ from their time-mean ($\overline{u}$ and $\overline{w}$, with overbar denoting the time-average), i.e., $u' = u - \overline{u}$, $w' = w - \overline{w}$, respectively. The sweeps are associated with the passage of coherent canopy-scale vortices, which form in the canopy shear layer. Specifically, for canopies of sufficient density, Raupach et al. (1996) demonstrated a similarity between canopy shear layers and free shear layers [47]. The drag discontinuity between the canopy and overflowing fluid leads to an inflection point, located near the top of the canopy, which triggers the Kelvin-Helmholtz (KH) instability that generates the coherent structures. The KH structures dominate the transfer of momentum to the canopy. For example, observations of aquatic [151] and terrestrial canopies [99] demonstrated that more than 80%–90% of the total downward momentum transport occurred within short, intense events that occupied only 25%–35% of total time. The dominating events occurred at time-intervals consistent with KH vortices. Scalar flux at the canopy interface has also been linked to the sweep events associated with KH vortices in both aquatic [101] and terrestrial canopies [102]. Because of the importance of these coherent structures to scalar and momentum exchange, it is vital that their intensity and depth of penetration into the canopy be properly modeled.

In this paper, a theoretical model based on a force balance for individual crosswind blades [3] (introduced in Section 4.2) is used to refine the model of velocity-dependent drag coefficient used in large-eddy simulation (LES) that parameterizes the effect of reconfiguration on airflow. A range of Vogel numbers can be identified to characterize different modes and degrees of reconfiguration, and their corresponding effects turbulence statistics are investigated for a maize canopy in Section 4.3. With mean vertical momentum flux constrained by field experimental data, increasingly negative $B$ shifts both the magnitude and vertical position of peak skewness and changes the distribution and strength of sweeps ($u' > 0$, $w' < 0$) and ejections ($u' < 0$, $w' > 0$). These results suggest that the proper modeling of turbulence in plant canopies requires that instantaneous reconfiguration be incorporated into
models through the use of a velocity dependent drag coefficient.

4.2 Theoretical Model of Reconfiguration

The theoretical model that predicts the impact of mean reconfiguration on the drag experienced by individual blades [3] can be used to infer the impact of instantaneous reconfiguration associated with the arrival of individual sweep events. The steady reconfiguration under steady (time-average) velocity \( \bar{u} \) can be quantified using an effective blade length, \( l_e \), which represents the length of a rigid, vertical blade that generates the same horizontal drag \( F_D \) as a flexible blade of total length \( l \) [3]. For blade width, \( b \), and fluid density, \( \rho \), the effective blade length \( l_e \) is given by the following definition,

\[
F_D = \frac{1}{2} \rho C_D^o b l_e U^2.
\]  (4.1)

In Eq. (4.1), the drag coefficient is assumed to be a constant, which is denoted by the superscript "o". Also note that, for generality, we use the characteristic velocity scale \( U \), which in this section refers to the time-averaged velocity \( \bar{u} \). Lutar and Nepf (2011) [3] used a numerical model to predict the total drag on a single blade \( F_D \), and from this they extract the ratio \( l_e/l \) as a function of the mean velocity \( \bar{u} \). As velocity increased, the blade bent over further in the streamwise direction, which decreased the frontal area and also created a more streamlined shape. Both effects are reflected in the decreasing value of \( l_e/l \). Many previous studies characterized reconfiguration of aquatic vegetation through changes in the drag coefficient [152], for which the total drag is,

\[
F_D = \frac{1}{2} \rho C_D U^2,
\]

with \( C_D \) a function of \( U \). Equating this drag expression to Eq. (4.1), one can show that \( l_e/l = C_D/C_D^o \sim U^B \), and we see that the dependence of \( l_e/l \) on \( U \) can be expressed through the Vogel exponent \( B \).

Blade posture in flow is governed by two parameters. The Cauchy number, \( Ca \), describes the ratio of the aerodynamic drag force to the restoring force due to rigidity. The dimensionless buoyancy, \( R_B \), described the ratio of restoring forces due to buoyancy and rigidity.

\[
Ca = \frac{1}{2} \frac{\rho C_D^o b U^2 l^3}{EI},
\]  (4.2)
Here, $\Delta \rho$ is the difference in density between the fluid and the blade, $g$ is the gravitational acceleration, $E$ is the elastic modulus, and $I = bt^3/12$ is the second moment of area, with $t$ the blade thickness. Because these two parameters control the blade posture in flow (i.e., the degree of bending), they also predict the dependence $l_e/l = C_D/C_D^0$, as described by Luhar and Nepf (2011) [3]. For example, Fig. 4.1(a) depicts the dependence of $C_D/C_D^0$ in the absence of buoyancy ($R_B = 0$, representing vegetation canopy elements in the atmosphere). For the lowest values of $Ca$, the blade remains essentially upright (negligible reconfiguration). Consistent with this posture, the drag is quadratic with $U$, i.e., $C_D/C_D^0 \approx 1$ and $B \approx 0$, similar to the response of the giant reed at low wind speed [129]. For $Ca > 100$, strong reconfiguration occurs (Fig. 4.1c), and the effective length-scale over which drag occurs ($l_e$) is comparable to the length-scale over which bending occurs ($l_b$).

For this degree of reconfiguration, specifically $l_b = l_e$, the balance of drag to the restoring force due to rigidity produces the scaling $l_e/l = Ca^{-1/3}$, $B = -2/3$, as previously derived by Alben et al. [2]. The drag coefficient ratio ($C_D/C_D^0$) displays this dependency in Fig. 4.1(a) for $Ca > 100$. Finally, for weak reconfiguration, associated with intermediate values of $Ca$ ($\approx 10$ to $50$), the blade is only slightly bent. In this posture (Fig. 4.1b), the effective length-scale for drag ($l_e$) is greater than the length-scale over which bending occurs ($l_b$) so that a balance of drag to rigidity yields the scaling $l_e/l = C_D/C_D^0 = Ca^{-1/3} (l_e/l_b)^2$, with $l_e/l_b > 1$. In this regime, as the velocity increases and the blade progressively bends further, $l_e/l_b$ decreases with increasing $Ca$, until $l_e/l_b \to 1$, at which point the regime of strong reconfiguration is reached. Within the weak reconfiguration regime, $(l_e/l_b)^2 \sim Ca^m$, and thus $l_e/l = Ca^{-(1/3+m)}$, $B = -(2/3 + 2m)$, so that $B$ is most negative in the weak reconfiguration regime. This feature was also observed for deforming plates and disks by Gosselin et al. (2010) [136]. In other words, for a blade geometry (i.e., bending in one dimension) the deviation from the quadratic drag response is greatest in the regime of weak reconfiguration. For example, in Fig. 4.1(a) the maximum slope occurs at $Ca = 21$, with $C_D/C_D^0 = Ca^{-0.54}$ (i.e., $B = -1.1$).

Finally, although the curves in Fig. 4.1(a) strictly describe steady reconfiguration under time-mean flow, we propose that the curves can be used to interpret the impact of reconfiguration on the drag experienced by individual sweeps penetrating...
the canopy. We anticipate that the highest skewness values will be observed in the weak reconfiguration regime, for which $B$ is the most negative, creating the greatest bias for strong events.

### 4.3 Numerical Simulation of Plant Reconfiguration

In this section we use a large-eddy simulation (LES) model to investigate the effects of different modes and degrees of plant reconfiguration on the turbulence characteristics inside a terrestrial canopy. The different modes and degrees of reconfiguration are modeled by varying the Vogel number $B$. We consider four cases: $B = 0$ (rigid canopy with no reconfiguration), $B = -2/3$ (strong reconfiguration for...
one-dimensional (1-D) linear elastic bending [2]), \( B = -1 \) (weak reconfiguration for 1-D elastic bending described in Section 4.2), and \( B = -4/3 \) (strong reconfiguration for two-dimensional (2-D) linear elastic bending [136]).

### 4.3.1 Numerical Model

The LES model employed here is described in detail by Pan et al. (2014) [5]. The drag force exerted by canopy elements per unit volume of air (\( f_D \)) is parameterized as a drag field following the approach proposed by the pioneer study of Shaw and Schumann (1992) [52],

\[
\mathbf{f}_D = -C_D (a_c \mathbf{P}) (|\mathbf{\tilde{u}}| \mathbf{\tilde{u}}),
\]

where \( \mathbf{\tilde{u}} \) is the filtered velocity, and \( a_c \) is the two-sided leaf area density. The projection tensor

\[ P = P_x \mathbf{e}_x \mathbf{e}_x + P_y \mathbf{e}_y \mathbf{e}_y + P_z \mathbf{e}_z \mathbf{e}_z \]

is used to split \( a_c \) into streamwise (\( x \)), spanwise (\( y \)), and vertical (\( z \)) directions, where \( \mathbf{e}_j \) is the unit vector in the \( j^{th} \) direction. Values of \( a_c \) and \( \mathbf{P} \) are provided by Pan et al. (2014) [5]. Please note the distinction between the volume average (\( f_D \)) and the drag on a single blade (\( F_D \)) defined by Eq. (4.1).

LES studies of forests [52–54,56,57,68] and crop canopies [55,123] typically treat \( C_D \) as a constant, i.e., \( \overline{C_D} \), implying \( |\mathbf{f}_D| \propto |\mathbf{\tilde{u}}|^2 \). To reflect the impact of reconfiguration, we adopt the general expression \( C_D = (U/A)^B \), with \( |\mathbf{\tilde{u}}| \) being the characteristic velocity scale \( U \). Here \( A \) is a velocity scale associated with canopy geometry and rigidity, and \( B \) is the Vogel number. The dependence of \( C_D \) on velocity can be estimated by fitting field experimental data to the mean momentum equation following the approach used by Cescatti and Marcolla (2004) [140]. Fitting \( C_D \) to data obtained in a large maize field near Mahomet, Illinois on July 10, 2011 (\( h = 2.1 \text{ m}, \text{LAI} = 3.3 \), and for details of field experiment see Gleicher et al. (2014) [4]), Pan et al. (2014) obtained \( A = 0.29 \text{ m s}^{-1} \) and \( B = -0.74 \) [5]. This estimated Vogel exponent is within the range of theoretical values (\( B = -2/3 \) to \(-4/3 \)) and other measured values (\( B = -0.5 \) to \(-0.8 \)), described in Section 4.1. Pan et al. [5] compared LES results using the drag model \( C_D = (|\mathbf{\tilde{u}}|/A)^B, A = 0.29 \text{ m s}^{-1}, B = -0.74 \) to results using a constant drag coefficient (\( C_D = 0.25 \), based on the data obtained by Wilson et al. (1982) [1]), which assumes no reconfiguration. The drag model that mimicked the impact of reconfiguration (\( B = -0.74 \)) produced a remarkable improvement in the comparison between LES results and observed
values of skewness (reducing the underprediction of $Sk_u$ and $Sk_w$ from 60% to 5% and 20%, respectively) and fraction of momentum carried by strong sweep events (reducing the underprediction from 40% to 5%).

In this work, an upper limit ($C_{D,\text{max}} = 0.8$, as suggested by experimental data) is used to cap the drag coefficient, reflecting the asymptotic regime of negligible reconfiguration in the limit of $\pi \to 0$. LES runs are conducted using the constant drag coefficient model ($C_D = 0.28$, $B = 0$; case (1)) and the revised reconfiguration drag model (velocity-dependent drag coefficient model),

$$C_D = \min \left( \left( |\tilde{u}|/A \right)^B, C_{D,\text{max}} \right),$$

considering a wide range of reconfiguration behavior, specifically, for cases (2) $A = 0.22 \text{ m s}^{-1}$, $B = -2/3$, (3) $A = 0.38 \text{ m s}^{-1}$, $B = -1$, and (4) $A = 0.48 \text{ m s}^{-1}$, $B = -4/3$. In each of these four cases the value of $B$ is prescribed, and the values of $C_D$ and $A$ are found by fitting the experimental data. Recall that an increasingly negative value of $B$ preferentially enhances the penetration of strong events into the canopy. In the fitting procedure each value of $C_D$ is weighted by the inverse of the velocity squared, so that higher weight is given to events of higher velocity, i.e., the conditions for which reconfiguration has the most impact on drag coefficient.

Fig. 4.2 compared drag coefficient models with experimental data. The revised velocity-dependent drag coefficient model presents a similar shape to the theoretical model depicted in Fig. 4.1(a). Beginning at 0.3 to 0.6 m s$^{-1}$, $C_D$ decreases with increasing velocity, and with higher dependence for more negative values of $B$. In particular, note that in the high velocity regime ($|\tilde{u}| > 1.5 \text{ m s}^{-1}$), $C_D$ decreases with increasingly negative value of $B$, corresponding to an increased tendency for reconfiguration to reduce the drag experienced by stronger events. However, for the low velocity regime ($|\tilde{u}| < 1 \text{ m s}^{-1}$), this trend is reversed, with $C_D$ larger for more negative values of $B$.

### 4.3.2 Simulation Results

LES results of turbulence statistics are compared with field experimental data computed using a period of 7.5 hours (0930-1700 CDT) of steady turbulence obtained on July 10, 2011 near Mahomet, Illinois (dots indicating the average and error bars indicating the standard deviation for 30-minute intervals in Figs. 4.3.
Figure 4.2. Drag coefficient \((C_D)\) against the magnitude of filtered velocity scale \((\tilde{u})\) fitted using field experimental data (circles) and the models \(C_D = \text{constant} \ (\text{grey line})\) and \(C_D = \min \left( \frac{(\tilde{u})}{A}, C_{D,\text{max}} \right) \) (Eq. (4.5); \(\text{black lines}\)). Grey solid and black solid, dash, and dash-dot lines indicate cases (1) \(C_D = 0.28 \ (B = 0)\), (2) \(A = 0.22 \text{ m s}^{-1}, \ B = -2/3\), (3) \(A = 0.38 \text{ m s}^{-1}, \ B = -1\), and (4) \(A = 0.48 \text{ m s}^{-1}, \ B = -4/3\), respectively.

and 4.4). Data obtained by Wilson et al. (1982) [1] (crosses in Fig. 4.3) are also shown to ensure the reliability of observations, because the canopy type and structure are similar in both datasets. In addition to vertical profiles of turbulence statistics, mechanisms of momentum transport inside the canopy are investigated using the quadrant analysis proposed by Lu and Willmarth (1973) [109]. Following the standard practices in LES studies, the mean stress \(\overline{u'w'}\) (and consequently the friction velocity \(u_* = \sqrt{\overline{|u'w'|}}\)) is determined using the resolved and subgrid-scale (SGS) parts. Standard deviations and skewness of velocity fluctuations are determined based only on the resolved scales. The vertical momentum flux is decomposed into four quadrants. Events in the first quadrant \((u' > 0, \ w' > 0)\) are outward interactions, events in the second quadrant \((u' < 0, \ w' > 0)\) are ejections, events in the third quadrant \((u' < 0, \ w' < 0)\) are inward interactions, and events in the fourth quadrant \((u' > 0, \ w' < 0)\) are sweeps [110]. Given a hole size \(H = |u'w'|/|\overline{u'w'}|\), \(S_{i,H}\) indicates the momentum flux carried by events in the \(i^{th}\) quadrant that satisfy \(|u'w'|/|\overline{u'w'}| > H\); \(S_{i,H} = S_{i,H}/|\overline{u'w'}|\) indicates the fraction of momentum flux carried by these events; and \(S_{H} = \sum_{i=1}^{4} S_{i,H}\) indicates the fraction of momentum flux carried by events in all four quadrants that satisfy \(|u'w'|/|\overline{u'w'}| > H\). In quadrant-hole analysis, the SGS component of the vertical momentum flux is excluded.
Figure 4.3. LES results of (a) normalized streamwise component of mean drag ($\bar{f}_{D,x}/(u^2_\tau/h)$), (b) normalized mean velocity ($\bar{u}/u_\tau$), (c) normalized mean Reynolds stress ($-\overline{w'w'}/u^2_\tau$), (d) ratio between sweeps and ejections ($S_{4,0}/S_{2,0}$), (e) normalized standard deviation of $u$ ($\sigma_u/u_\tau$), (f) normalized standard deviation of $w$ ($\sigma_w/u_\tau$), (g) skewness of $u$ ($Sk_u$), and (h) skewness of $w$ ($Sk_w$) against normalized height ($z$). Here $u_\tau$ is the friction velocity, and $h$ is the canopy height. Simulation results (lines, see Fig. 4.2 for representations) are evaluated against field experimental data (symbols). Dots with error bars indicate average and standard deviation for 30-minute intervals of data obtained during 0900-1730 CDT on 10 July 2011 in a large maize field near Mahomet, Illinois [4,5], and crosses indicate data obtained by Wilson et al. (1982) [1]. The canopy type and structure are similar in both datasets.

Figure 4.4. Comparison of LES results and field experimental data of fractions of vertical momentum flux carried by (a) all events ($S_{fH}$), (b) ejections ($S_{2,H}$), and (c) sweeps ($S_{4,H}$) against hole size ($H$) at $z/h = 2/3$. See Fig. 4.3 for representations of lines and symbols.
In Fig. 4.3(a), predictions of the streamwise component of time-averaged drag, $f_{D,x}$, is negative for all four cases. The vertical integration of $f_{D,x}$ is held approximately constant (with less than 0.5% difference across all cases), because parameters in the model $C_D = C_D(\bar{u})$ (i.e., $A$ and $B$ in Eq. (4.5)) are fitted using the measured profile of mean vertical momentum flux (see Fig. 4.2). Increasingly negative values of $B$ decreases the magnitude of $f_{D,x}$ in the upper 20% of the canopy, the region belonging to the high velocity regime, and increases the magnitude of $f_{D,x}$ in the lower 80% of the canopy, the region belonging to the low velocity regime. In Fig. 4.3(b), predictions of normalized, time-mean velocity, $u/\bar{u}_h$, resulting from drag models with $B \neq 0$ (black lines) are distinct from those with $B = 0$ (gray line), showing better agreement with measurements inside the canopy. Specifically, using an average $C_D$ (assuming $B = 0$, no reconfiguration) produces an overestimation of the mean velocity inside the canopy by 100%, suggesting an underestimation of $f_{D,x}$ in the lower 80% of the canopy. For second-order moments, increasingly negative values of $B$ only slightly increases the downward momentum flux ($|u'w'|$; Fig. 4.3c) and the standard deviation of $u$ ($\sigma_u$; Fig. 4.3e). In other words, ignoring the effect of reconfiguration by assuming a constant $C_D = \overline{C}_D$ leads to only a slightly shallower estimation of the penetration of momentum into the canopy layer, consistent with the findings of Wilson et al. (1982) [1]. The effects of reconfiguration on the standard deviation of $v$ ($\sigma_v$; not shown) and $w$ ($\sigma_w$; Fig. 4.3f) are negligible, implying that reconfiguration affects mostly the energy contained in the streamwise direction rather than spanwise or vertical directions.

The effects of the mode of reconfiguration, characterized by the negative value of $B$, are most pronounced for the sweep-ejection ratio ($S_{4,0}/S_{2,0}$; Fig. 4.3(d)) and the skewness of $u$ ($Sk_u$; Fig. 4.3g) and $w$ ($Sk_w$; Fig. 4.3h), with the magnitude of all three statistics increasing with increasingly negative $B$. The increasing magnitude of skewness arises directly from the reduction in drag coefficient with increasing velocity, which, as mentioned in Section 4.1, allows stronger events to penetrate more easily into the canopy. For example, at $z/h = 2/3$, the fraction of vertical momentum flux carried by events eight times stronger than the mean magnitude ($H = 8$) increases from 27% for $B = 0$ to 50% for $B = -1$ (Fig. 4.4a). As $B$ becomes more negative, the deeper penetration of stronger events also makes the peak of $Sk_u$ move towards the ground (Fig. 4.3g). Sweep events are associated with elevated streamwise velocity ($u' > 0$), and thus receive a preference in regimes
for which \( C_D \) decreases with increasing \( U \), and thus become stronger when \( B \) is more negative. At \( z/h = 2/3 \), for example, the fraction of vertical momentum flux carried by sweep events increases from 75\% (\( B = 0 \)) to 85\% (\( B = -1 \)) for \( H = 0 \) and from 25\% (\( B = 0 \)) to 50\% (\( B = -1 \)) for \( H = 8 \) (Fig. 4.4c). On the other hand, ejection events associated with weaker streamwise velocity (\( u' < 0 \)) are preferentially damped in this regime, and thus become weaker when \( B \) is more negative. At \( z/h = 2/3 \), for example, the fraction of vertical momentum flux carried by ejection events decreases from 50\% (\( B = 0 \)) to 35\% (\( B = -1 \)) for \( H = 0 \) and from 15\% (\( B = 0 \)) to negligible (\( B = -1 \)) for \( H = 4 \) (Fig. 4.4b). The increase in sweeps and decrease in ejections both lead to the increase in the sweep-ejection ratio (Fig. 4.3c). The overall best agreement with observations across skewness and quadrant analysis occurs for \( B = -1 \) (black dash lines in Figs. 4.3d, g, h and 4.4). Note that when \( B \) is fitted to data, Pan et al. (2014) [5] obtained \( B = -0.74 \). However, as seen in Fig. 4.2, the points calculated from the data do not constrain the fit very tightly. A new fit, which more heavily weights the large velocity portion of the data (which is more reliably measured in the field), yields \( B = -0.83 \). The idea that the reconfiguration of the maize plants falls in the regime of weak reconfiguration for the 1-D elastic case (described in Section 4.2) seems perfectly reasonable, because the simple bending observed in the field does not display deflection beyond the posture in Fig. 4.1(b).

### 4.4 Conclusions

Results obtained from laboratory and numerical experiments demonstrate that concepts developed for mean reconfiguration can be extended to instantaneous reconfiguration, at least for time-scales over which the plant can respond. This provides a link between plant reconfiguration and turbulence dynamics. In particular, as the values of Vogel number becomes more negative, the peak \( Sk_u \) increases in magnitude. Specifically, LES of a maize canopy gives \( Sk_{u,\text{max}} \) of 0.8, 1.3, and 1.8 when \( B \) is specified to be 0, −2/3, and −1, respectively (Fig. 4.3g). In addition, deeper penetration of stronger sweep events (lower values of \( z (Sk_{u,\text{max}} / h) \)) is observed when these events are more preferentially allowed by reconfiguration (larger values of \( Sk_{u,\text{max}} \)), as inferred from Fig. 4.3(d). Note that we do not imply that reconfiguration is the only mechanism that affects skewness. For example, in
a canopy of steel cylinders (no reconfiguration) the value of $S_{k_{u,\text{max}}}$ increased from negligible to 0.8 when LAI was increased from 0.03 to 0.5 [49]. In an orchard forest canopy, the value of $S_{k_{u,\text{max}}}$ decreased from 1 to negligible when the atmospheric temperature stratification condition changed from neutral to free convection [97]. Our results show that, if other conditions remain unchanged, more negative values of $B$ will cause more penetration of sweeps and larger values of $S_{k_u}$.

For one-dimensional linear elastic reconfiguration, we highlight the importance of weak reconfiguration, which is the transition between the asymptotic regimes of negligible reconfiguration ($B = 0$) and strong reconfiguration ($B = -2/3$). In the weak reconfiguration regime, the bending length-scale is smaller than the drag length-scale, leading to a stronger dependence between drag coefficient and velocity than that observed during strong reconfiguration. In other words, the Vogel exponent is more negative ($B < -2/3$) in the weak reconfiguration regime, reaching a peak value of $B = -1.1$ at $Ca = 21$. Importantly, because weak reconfiguration produces the most negative Vogel exponents, it also produces the strongest impact on skewness. All three regimes, including weak reconfiguration, are likely present in natural canopies in which simple bending is observed, like seagrasses, stems, branches, maize, and wheat. Gosselin et al. [136] described a similar intermediate regime of bending for plates and disks. For strong reconfiguration, the Vogel exponent has been shown to be more negative for 2-D bending ($B = -4/3$) than for 1-D bending ($B = -2/3$) [2,137] and, as our LES results show, the 2-D regime results in the largest predictions of skewness. A wide range of broad leaves can fold into cones and experience 2-D reconfiguration, and thus enter the $-4/3$ regime [153]. Many terrestrial canopies have a Vogel number between $-2/3$ and $-4/3$ [135,137].

With the vertically integrated mean drag force held approximately constant, changing the mode of the reconfiguration has a strong impact on the mechanisms of momentum transport. The mean momentum flux remains the same, but the distribution, strength, and fraction of momentum carried by sweeps and ejections is altered significantly. This result suggests that different canopies, with different reconfiguration geometries, will affect the flow structure in different ways. The current understanding of canopy turbulence is based on relating the properties of coherent structures to the mean drag force exerted by the canopy (one example is the penetration depth studied by Ghisalberti and Nepf (2006) [151]). Perhaps further advances will result from understanding the drag reduction by reconfiguration and
its effects on instantaneous turbulence structure. This paper shows that higher order moments such as skewness, as well as the fractions of momentum transported by sweeps and ejections, are very sensitive to reconfiguration.
Chapter 5 | Dispersion of Particles Released from Canopy Edge

5.1 Introduction

Most of the studies associated with turbulence and particle dispersion inside and above plant canopies are conducted for horizontally extensive and uniform canopy [1, 4, 5, 52–57, 68, 144]. A recent large-eddy simulation (LES) study has successfully reproduced turbulence statistics up to the third order and the three-dimensional (3-D) mean particle concentration field during a point-source released experiment conducted in the interior of a large maize field [5]. However, the land surface is a patchwork of vegetation and land use composed of many different surfaces. In many landscapes these patched are small, and therefore a great portion of these landscapes are field edges. Understanding the transport processes in canopy edge flows is critical for interpreting flux measurements of sensible and latent heat, greenhouse gases, and air pollutants [154], as well as estimating the dispersal of biogenic particles such as pollens [13] and spores [71]. Specifically, measurements suggest that pathogenic fungal spores released at the canopy leading edge tend to disperse farther than those released in the field interior [71], and therefore infections at the canopy edges may be more likely to initiate disease epidemics than those in the field interior.

Turbulent flows downstream from canopy leading edges have been studied using field [74–76] and wind tunnel [72, 73] measurements, theoretical models [8], and large-eddy simulation (LES) models [7, 56, 69, 70, 77]. The leading edge flow can be
divided into distinct regions based on flow characteristics. The theoretical model of Belcher et al. (2003) proposed five distinct regions based on the characteristics of mean flow and downward momentum flux: (1) the *impact region* located upwind from the edge, (2) the *adjustment region* within the canopy downstream from the edge where the flow is decelerated by canopy drag, (3) the *canopy interior region* where the canopy drag is balanced by downward momentum flux, (4) the *canopy shear layer* at the canopy top where coherent structures develop, and (5) the *roughness-change region* above the canopy where the internal boundary layer (IBL) develops (see Fig. 3 in Beltcher et al. (2003) [8]). In this model, an important length scale is the canopy-drag length scale, representing the streamwise distance required for canopy to consume kinetic energy from an air parcel. This length scale was used to estimate the distance within the canopy for the flow to adjust to the canopy drag [8,155]. LES results of Dupont et al. (2009) suggested four stages for the development of coherent structures near the canopy leading edge: (1) close to the edge Kelvin-Helmholtz (KH) instabilities develop at the canopy top due to drag discontinuity, (2) the KH instabilities roll over to form transverse vortices, (3) secondary instabilities destabilize these rollers and two counter-rotating streamwise vortices appear, and (4) the initial rollers have become complex three-dimensional coherent structures with spatially constant mean length and separation length scales [7]. The authors used a length scale proportional to the depth of the IBL to characterize the distance occupied by coherent structures in each stage of development. Note that this length scale can also be related to the canopy-drag length scale, because stages develop closer to the edge with increasing canopy density [7]. The distinct flow characteristics in different regions near the edge may lead to different behavior of particle dispersion. For example, the deceleration of mean streamwise velocity in the *adjustment region* induces positive mean vertical velocity due to continuity, whereas positive mean advection is absent in the *canopy interior region*. The size and penetration depth of coherent structures can modify the turbulent transport mechanism within the canopy, which also affects particle transport near the field edge.

The objective of this work is to investigate the effect of canopy leading edge on the dispersion of particles released from points sources inside the canopy. The LES model is described in Section 5.2. The adjustment of the flow above and within the canopy is analyzed in Section 5.3, where the adjustment distances for mean flow,
TKE, and coherent structures are studied. The effects of distance of the source from the canopy leading edge on the dispersion of particles are investigated in Section 5.4. Conclusions follow in Section 5.5.

5.2 Numerical Model

The LES model employed in this work was described in detail in Chapters 3 [5] and 4 [11]. The model solves the 3-D momentum equation using a fully dealiased pseudo-spectral approach in horizontal directions and a second-order centered finite-difference scheme in the vertical direction. The equations are closed using the Lagrangian scale-dependent dynamics Smagorinsky subgrid-scale (SGS) model. Particle dispersion is treated using an Eulerian approach. The conservation of particle mass is discretized using a finite-volume scheme with a third-order bounded scheme for the advection term [80]. Following Chamecki and Meneveau (2011) [92], the advective velocity for the particle concentration field is approximated as the superposition of the instantaneous fluid velocity and a constant particle settling velocity ($w_s = 0.0194$ m s$^{-1}$ for Lycopodium spores [5]). The effect of particle inertia is neglected due to small Stokes numbers considered in the simulations [12]. The SGS particle flux is modeled using an eddy-diffusivity approach and a constant SGS Schmidt number ($Sc_{SGS} = 0.4$) [81]. Following the pioneer LES study of Shaw and Schumann (1992) [52], the effect of canopy elements on the flow field is parameterized as a drag force term in the momentum equation using a drag coefficient, the projected leaf area density, and the filtered velocity [5]. In this work, the model $C_D = \min((|\tilde{u}|/A)^B, C_{D,max})$ was used for drag coefficient, where $\tilde{u}$ is the filtered velocity, $A = 0.22$ m s$^{-1}$ is a velocity scale associated with plant geometry and rigidity, $B = -2/3$ is the Vogel number associated with strong reconfiguration for one-dimensional linear elastic bending, and $C_{D,max} = 0.8$ is the upper limit of $C_D$ for maize canopy elements [11]. The rate of particle deposition on canopy elements is estimated using a modified version of the model described by Aylor and Flesch (2001) [67] (see Appendix A [5] for details).

A total of 12 LES runs were performed to study turbulence and particle dispersion downstream from a canopy leading edge. The simulation domain is a box with $L_x \times L_y \times L_z = 44.3h \times 20h \times 10h$ descritized using $186 \times 84 \times 120$ grid points respectively, where $h = 2.1$ m is the maize canopy height. The modeled canopy
occupies $24h$ of the streamwise domain (grid points 34–135), the entire spanwise
domain ($L_y$), and the first 12 vertical layers. For the flow field, a no-stress boundary
condition is imposed at the top of the domain. Note that the no-stress boundary
condition at this height ($10h$) is unrealistic, but this detail is not expected to impact
turbulence statistics within the canopy layer and the IBL (the region of the flow
strongly modified by the presence of the plant canopy) [5,108]. A wall model is used
to parameterize the bottom boundary condition at the ground beneath the plants
(the roughness length $z_0 = 0.01\, \text{m}$). An inflow boundary condition at the beginning
of the domain is provided by a precursor simulation of the same configuration
except that the plant canopy is absent. The inflow is imposed at $8h$ upstream
from the canopy leading edge, a location unlikely to be affected by the downstream
plant canopy. The last $4h$ of the domain (grid points 169–186, beginning $8.3h$
downstream from the canopy trailing edge) is used as a fringe region [156] to force
the velocity field back to the inflow, which allows us to simulate non-periodic flow
in the streamwise direction using pseudospectral numerics. The spin-up of the flow
field consists of a first stage of 32 minutes for fully development of in the absence
of the canopy, a second stage of 40 minutes for mean flow and turbulence to adjust
to the presence of the canopy patch and reach statistically steady state using inflow
produced by the precursor simulation. After the same spin-up, each case study of
particle dispersion is conducted for 1.2 hours with inflow produced by the precursor
simulation. Particles were released from point sources at streamwise locations
$x_{src}/h = 0, 1.9, 9, \text{ and } 13.6$, and vertical locations at $z_{src}/h = 1, 2/3, \text{ and } 1/3$ for
each $x_{src}$. The analysis of results is based on the last hour of each LES case study,
and thus approximates statistically steady-state conditions for the concentration
field. The flow field and particle dispersion were analyzed for $-4 < x/h < 20$ (from
the impact region to canopy interior region with fully developed three-dimensional
coherent structures, but not affected by the canopy trailing edge at $x/h = 24$),
$0 < z/h < 4$ (including the canopy layer and the IBL, but not affected by the
unrealistic no-stress top boundary condition at $z/h = 10$). The streamwise source
location ($x_{src}/h$) and the domain for analysis of results are specified based on the
characteristics of the flow field identified in Section 5.3.
5.3 Flow Field Downstream From the Canopy Leading Edge

Above the canopy ($z/h > 1$) the adjustment of mean flow to the change of surface roughness is characterized by the development of an internal boundary layer (IBL) (calculated as the region $\partial \bar{u}/\partial z - (\partial \bar{u}/\partial z)_{\text{inf}} > 0$ [6,7], where subscript inf indicates results for the infinite canopy case from Pan et al. (2014) [5]; Fig. 5.1). The region of the flow strongly modified by the presence of the canopy (including the canopy layer and the IBL) is well confined within the region $0 < z/h < 4$ used for analysis of results. The depth of IBL becomes comparable with the canopy height at $x/h = 6$ and reaches two canopy heights at $x/h = 20$ (where the IBL is still growing), consistent with the results obtained by [7].

Within the canopy ($z/h < 1$), the streamwise velocity ($\bar{u}$; Fig. 5.2a) decelerates as a consequence of canopy drag, transforming from a boundary-layer type mean wind profile at the canopy leading edge ($x/h = 0$) to a canopy-shear-layer type inflected mean wind profile in the field interior ($x/h \gg 1$). The mean flow is considered fully adjusted to the canopy drag when the streamwise gradient of $\bar{u}$ within the canopy becomes negligible ($|\partial \bar{u}/\partial x| < 0.1$; white region in Fig. 5.2b). The adjustment distance for $\bar{u}(z/h < 1)$ is longer than the theoretical estimate of $3L_c$ [155] (here $L_c$ is the canopy-drag length scale), especially in the lower canopy.

Figure 5.1. Iso-contours of $\partial \bar{u}/\partial z - (\partial \bar{u}/\partial z)_{\text{inf}}$ normalized by $u_*/h$ plotted in $x/h$ (downwind) and $z/h$ (vertical) space. The development of IBL is calculated as the region $\partial \bar{u}/\partial z - (\partial \bar{u}/\partial z)_{\text{inf}} > 0$ above the canopy ($z/h > 1$) [6,7].
region \((z/h < 1/2)\), consistent with the results obtained by Dupont et al. (2009) \[7\]. Specifically, the adjustment distance for \(\tau\) reaches \(x/h = 16\) near the ground \((z/h \to 0; \text{Fig. 5.2b})\). From continuity, the deceleration of \(\tau\) leads to positive mean vertical velocity \((\bar{w} > 0)\) within and above the canopy for \(x/h < 14\) (Fig. 5.2c). Close to the edge \((-0.2 < x/h < 1.2)\), weak acceleration of \(\tau\) \((\partial\tau/\partial x > 0; \text{Fig. 5.2b})\) and consequent negative mean vertical velocity \((\bar{w} < 0; \text{Fig. 5.2c})\) are observed in the region near the ground \((z/h < 1/2)\), because the region with high leaf area density \((0.3 < z/h < 0.9; \text{Table 3.1})\) behaves like an obstacle in the flow. Close to the canopy trailing edge \((x/ = 24)\), the acceleration of \(\tau\) induces negative mean vertical velocity \((\bar{w} < 0)\) at \(x/h > 15\), but within the canopy this effect is negligible for \(x/h < 20\) \(|\bar{w}|/u_\ast < 0.1; \text{Fig. 5.2c}\). In other words, the canopy trailing edge at \(x/h = 24\) is unlikely to affect the flow field within the canopy for \(x/h < 20\).

Vertical transport of particles near the edge consists of mean advection and turbulent dispersion. Vertical turbulent transport depends on the vertical component of TKE \((\sigma_w^2)\). Fig. 5.3(a) shows that \(\sigma_w\) at a given height within the canopy \((z/h < 1)\) becomes nearly independent of downstream distance from the leading edge at \(x \approx 6L_c = 10.8h\), where \(6L_c\) is the adjustment distance for TKE estimated by Belcher et al. (2008) \[155\] based on laboratory measurements obtained by Morse et al. (2002) \[73\]. The relative importance of mean and turbulent transport in the vertical direction can be ascertained using the ratio \(\bar{w}/\sigma_w\) (Fig. 5.3b). The effect of mean vertical velocity may be neglected within the region where \(|\bar{w}|/\sigma_w < 0.1\) \((\text{white region in Fig. 5.2b})\). This effect is discussed further in Section 5.4.

The drag discontinuity between the canopy and the overflowing fluid leads to an infection point located near the canopy top for the profile of mean streamwise velocity \((\bar{u}(z))\). This infection point triggers Kelvin-Helmholtz (KH) instability that generates eddies of sizes characterized by the shear length scale, \(L_s = u_h/(\partial\bar{u}/\partial z)_h\), where subscript \(h\) indicates values at the canopy top \[47\]. Downstream from the canopy leading edge, the shear length scale decreases from \(L_s/h \approx 1\) at \(x/h = 0\) to a minimum at \(x \approx L_c\). It then increases slowly with downwind distance \((1 - L_s)/h\) reaching a maximum at \(x \approx L_c\) and then decreases slowly with \(x\); dash line in Fig. 5.4), consistent with results obtained by Dupont et al. (2009) \[7\]. It should be noted that \(L_s\) defined using mean flow properties may not be a robust measure of the development of KH coherent structures because the penetration of strong sweep events associated with KH coherent structures into the canopy
is changeable without modifying first- and second-order turbulence statistics [11]. Both laboratory measurements and LES results suggest that a better measure of the penetration depth of KH coherent structures is the position of peak streamwise velocity skewness inside the canopy \((z(S_{u,\text{max}}))\) [11]. When boundary layer winds approach the canopy leading edge, an abrupt jump of \(z(S_{u,\text{max}})\) from the ground to the canopy top is observed at \(x \approx L_c\) (solid line in Fig. 5.4), consistent with the downstream distance required for the formation of canopy-scale eddies [7]. For \(x < L_c\), formation of canopy-scale eddies may be suppressed due to the suppression of TKE within the canopy [69,70] (e.g., \(\sigma_w(z/h<1)\) decreases with downstream distance at \(x < L_c\); Fig. 5.3(a)). At \(x > L_c\), \(z_{S_{u,\text{max}}}\) decreases with \(x/h\) until reaching a constant value at \(x/h \geq 13.3\) (solid line in Fig. 5.4, where abrupt decreases in the solid line are due to a vertical grid size of \(h/12\)), implying that KH coherent structures grow and increase their penetration before reaching a fully developed state at \(x/h \geq 13.3\).

Within the canopy, different adjustment distances are observed for mean flow (e.g., \(x/h \approx 16\) for \(\overline{u}\) from Fig. 5.2(b), \(x/h \approx 12.3\) for \(\overline{w}\) from Fig. 5.2(c)), TKE (e.g., \(x/h \approx 10.8\) for \(\sigma_w\) from Fig. 5.3(a)), and coherent structures (e.g., \(x/h \approx 13.3\) for \(z(S_{u,\text{max}})\) from Fig. 5.4). Fig. 5.5 compares profiles of turbulence statistics at \(x/h = 13.3\) (dash lines), 16 (solid lines), and 20 (dash-dot lines) with those in the field interior (dots; [5]). Profiles at these three locations collapse and agree well with those in the field interior for mean streamwise velocity \((\overline{u}; a)\), mean Reynolds stress \((\overline{uw}; b)\), the ratio between Reynolds stress carried by sweeps and ejections \((S_{4,0}/S_{2,0}; c)\), standard deviations of streamwise \((\sigma_u; d)\), spanwise \((\sigma_v; e)\), and vertical \((\sigma_w; f)\) velocities, as well as skewness of streamwise \((S_{u,\text{max}})\) and vertical \((S_{w,\text{max}})\) velocities. These results suggest that mean streamwise advection and turbulent dispersion within the canopy are fully developed at \(x/h > 13.3\), and particles released at \(x_{\text{src}}/h > 13.3\), \(z_{\text{src}}/h < 1\) should be transported in a similar pattern to those released from the field interior as long as mean vertical advection is negligible \((|\overline{w}|/\sigma_w < 0.1)\). At \(z/h = 13.3\), however, non-negligible positive mean vertical velocity \((\overline{w}/\sigma_w > 0.1)\) observed at \(z/h < 1/2\) (dash line in Fig. 5.5g) can affect vertical transport of particles within the canopy, and this effect is expected to be enhanced for particles released in the bottom half of the canopy.

Above the canopy \((z/h > 1)\), the most apparent difference between the profiles at \(13.3 < x/h < 20\) and those in the field interior is the reduction of \(\sigma_u\) (lines
compared with *dots* in Fig. 5.5d), because the streamwise component of TKE ($\sigma_u^2$) is primarily produced by shear [70], and is therefore sensitive to the depth of IBL. The vertical component of TKE ($\sigma_w^2$), on the other hand, is primarily produced by pressure redistribution, and therefore within the canopy the adjustment of $\sigma_w^2$ downstream from the leading edge ($x/h < 0$) starts later than $\sigma_u^2$ but reaches its fully developed state faster than $\sigma_u^2$ [70]. The profiles of $\sigma_w$ at $13.3 < x/h < 20$ are almost identical as those in the field interior (*lines* compared with *dots* in Fig. 5.5f).

### 5.4 Effects of Canopy Leading Edge on Dispersion of Particles

Figs. 5.6–5.9 depict the spatial distribution of mean concentration integrated in crosswind direction ($\chi(x,z) = \int_y \overline{C} dy$ normalized by the point source strength ($Q$), where $\int_y$ indicates integration from $y \rightarrow -\infty$ to $y \rightarrow \infty$) for particles released at four streamwise locations ($x_{src}/h = 0, 1.9, 9, \text{ and } 13.6$) and three heights ($z_{src}/h = 1, 2/3, \text{ and } 1/3$). The four streamwise locations correspond to the canopy leading edge ($x/h = 0$), the development of canopy-scale eddies ($x \geq L_c = 1.8$), the transition region ($L_c/h < x/h < 13.3$), and the region with fully developed turbulence structures ($x/h > 13.3$), as discussed in Section 5.3. The extension in the downstream direction of the iso-contour of $\chi/Q = 0.1$ s m$^{-2}$ presents a peak at the canopy top ($z/h = 1$) for all cases, and an additional peak at the ground ($z/h = 0$) for particles released in the bottom half of the canopy ($z_{src}/h = 1/3$). The downwind distance from the source ($x - x_{src}$) to which the iso-contour of $\chi/Q = 0.1$ s m$^{-2}$ stretches is a measure of the dispersal distance of particles. For example, for $z_{src}/h = 1/3$, the iso-contours of $\chi/Q = 0.1$ s m$^{-2}$ reach ($x - x_{src}$)/$h \approx 14, 14, 7$, and 3 for particles released at $x_{src}/h = 0, 1.9, 9, \text{ and } 13.6$, respectively (Figs. 5.6c, 5.7c, 5.8c, and 5.9c), supporting observations that particles released at the canopy leading edge tend to disperse farther than those released in the field interior [71].

The growth of the particle plume can be inferred from the stretch of the iso-contour $\chi/Q = 0.1$ s m$^{-2}$ in the vertical direction. Specifically, for particles released at $x_{src}/h < 2$, $z_{src}/h \geq 2/3$, the arched iso-contours of $\chi/Q = 0.1$ s m$^{-2}$ (Figs. 5.6a, b and 5.7a, b) demonstrate the effect of positive mean vertical velocity ($\overline{w} > 0$) at the canopy leading edge (Fig. 5.2c). Quantitatively the growth of the plume can
be characterized by the mean height (dots in Figs. 5.6–5.9),

\[ \bar{z}(x) = \frac{\int_{z=0}^{\infty} z \chi(x, z) \, dz}{\int_{z=0}^{\infty} \chi(x, z) \, dz}, \]  

and the mean depth,

\[ \sigma_z(x) = \left( \frac{\int_{z=0}^{\infty} (z - \bar{z})^2 \chi(x, z) \, dz}{\int_{z=0}^{\infty} \chi(x, z) \, dz} \right)^{1/2} = (\bar{z}^2 - \bar{z}^2)^{1/2}. \]  

For each case most particles are confined to the region \( \bar{z} \pm \sigma_z \) (between two dash lines in Figs. 5.6–5.9). The location of maximum integrated mean concentration (\( \chi \)) coincides with the centroid of the plume (\( \bar{z} \)) within a limited downstream distance from the source, and then deviates from \( \bar{z} \) as the plume becomes increasingly skewed (plus signs compared with dots in Fig. 5.6–5.9). For all cases, the location of maximum \( \chi \) at a given \( x \) (\( z_{\text{max}} \)) sits at \( z/h = 1 \) away from the source (e.g., at \( x/h > 16 \) for \( x_{\text{src}} \leq 13.6 \)), consistent with the peak of the downstream stretch of the iso-contour \( \chi/Q = 0.1 \, \text{s m}^{-2} \). For \( z_{\text{src}}/h = 1/3 \), an abrupt jump of \( z_{\text{max}} \) from the ground to the canopy top occurs at \( x - x_{\text{src}}/h \approx 14, 11.5, 5.5, \) and 3.3 for particles released at \( x_{\text{src}}/h = 0, 1.9, 9, \) and 13.6, respectively (plus signs in Figs. 5.6c, 5.7c, 5.8c, and 5.9c), consistent with the existence of two peaks of the downstream stretch of the iso-contour \( \chi/Q = 0.1 \, \text{s m}^{-2} \).

Comparisons of \(\bar{z}(x - x_{\text{src}}) \) and \(\sigma_z(x - x_{\text{src}}) \) for particles released from different locations (\( x_{\text{src}}, z_{\text{src}} \)) suggest that both \( \bar{z} \) and \( \sigma_z \) become independent of \( z_{\text{src}} \) at \( (x - x_{\text{src}})/h \approx 15, 13, 6, \) and 3 for particles released at \( x_{\text{src}}/h = 0, 1.9, 9, \) and 13.6, and are likely to become independent of \( x_{\text{src}} \) at \( (x - x_{\text{src}})/h > 16 \) (red, green, cyan, and blue lines at in Fig. 5.10). The collapse of \( \bar{z} \) and \( \sigma_z \) suggests that the particle plumes at \( x/h > 16, z/h > 1 \) scaled by the strength of the plume should yield the same plume geometry, and therefore the effects of the canopy leading edge on the dispersion of particles can be separated into effects on the plume strength and geometry. The downstream distances \( (x - x_{\text{src}}) \) required for \( \bar{z} \) to become independent of \( z_{\text{src}} \) are comparable with those for the abrupt jump of \( z_{\text{max}} \) for particles released at \( z_{\text{src}}/h = 1/3 \). For particles released from the field interior, both \( \bar{z} \) and \( \sigma_z \) become independent of \( z_{\text{src}} \) and display a power-law dependence on \( x - x_{\text{src}} \) once the transition to \( z_{\text{max}}/h = 1 \) is reached, while the growth rates (the power-law exponents) are enhanced by eddy-diffusivity and reduced by mean
shear [5]. For particles released close to the canopy edge, the transport of particles within the IBL experience greater mean shear than those above the field interior \((\partial \bar{u} / \partial z - (\partial \bar{u} / \partial z)_{\text{inf}} > 0; \text{Fig. 5.1})\). Consequently, the growth rates of collapsed \(z\) and \(\sigma_z\) when most of airborne particles are located within the IBL (see discussions below) are slower than those for the infinite canopy case (color lines compares with black lines in Figs. 5.10). In other words, the canopy leading edge affects the geometry of the plume through the development of the IBL.

The strength of the plume can be characterized using the fraction of particles that remain airborne and escape the canopy, calculated as \(AF = \int_x \int_{z=h}^{\infty} \int_y u C dy dz dx\) and \(EF = \int_x \int_{z=0}^{\infty} \int_y u C dy dz dx\) respectively, where \(\int_x\) indicates integration from \(x \to -\infty\) to some arbitrary \(x\) [5]. For all cases in this work, most of the airborne particles at \(x/h > 16\) are located above the canopy (EF/AF > 0.9; Fig. 5.11b) and within the IBL (\(z + \sigma_z\) located within the region that \(\partial \bar{u} / \partial z - (\partial \bar{u} / \partial z)_{\text{inf}} > 0\) in Fig. 5.1). Therefore away from the source, the strength of the plume can be calculated as a product of the source strength \((Q)\) and the escape fraction \((EF)\). The escape fraction can be estimated as \(EF \approx 1 - F_{Sp} - F_{SG}\), where \(F_{Sp}\) and \(F_{SG}\) are the fractions of particles removed by deposition on canopy elements and the ground, respectively, and \(1 = AF + F_{Sp} + F_{SG}\) from the conservation of particle mass.

The canopy deposition model described in Appendix A assumes that rebound and re-entrainment of particles occur when the instant horizontal velocity \((\sqrt{\bar{u}^2 + \bar{v}^2})\) is greater than a critical value \((V_{crit} = 0.45 \text{ m s}^{-1})\). Therefore deposition on canopy elements is unlikely to occur when the magnitude of mean streamwise velocity \((|\bar{u}| \approx \sqrt{\bar{u}^2 + \bar{v}^2})\) is greater than \(V_{crit}\) (within the region that \(\bar{u}/u_* \geq 1\) in Fig. 5.2a given \(u_* \approx V_{crit}\) in this work). Consequently, results of \(F_{Sp}\) show that particles do not deposit on canopy elements at \(x/h < 4\) (Fig. 5.12a). Despite the highly empirical canopy deposition model described in Appendix A, these results suggest that in the scenario of wind blowing from flat, bared landscapes to a single type of crops, field edges may be less likely to be infected by spores from distant locations than the field interior. Therefore scouting of infections around the edge of the field may be insufficient to monitor the health of crops. The retention and re-entrainment of particles can be suppressed for wet canopy elements (with the presence of dew), a case beyond the scope of this work that plays a critical role in the initiation of disease epidemics [35]. Within the canopy interior region where mean streamwise
velocity has adjusted to the canopy drag ($|\partial u/\partial x|/(u_*/h) < 0.1$; white region in Fig. 5.2b), the probability for rebound and re-entrainment should behave similarly to that in the field interior. In addition, within the region that $|\overline{u}|/V_{\text{crit}} \ll 1$ (i.e., $|\overline{u}|/u_* < 0.1$; white region in Fig. 5.2a), changes in the mean streamwise velocity are unlikely to modify the probability for rebound and re-entrainment. Consequently, particles released at $x_{\text{src}}/h = 13.6$ yield approximately the same $F_{S_p}$ as those for the case of infinite canopy (blue and black lines in Fig. 5.12a). Within the overlap region of $|\partial u/\partial x|/(u_*/h) > 0.1$ in Fig. 5.2(b) and $|\overline{u}|/u_* > 0.1$ in Fig. 5.2(a), deposition on canopy elements is suppressed due to increased probability for rebound and re-entrainment. This effect is enhanced with decreasing downstream distance from the canopy edge. Consequently, for a given $z_{\text{src}}$, particles released away from the edge (large $x_{\text{src}}$) yield higher $F_{S_p}(x-x_{\text{src}})$ than those released close to the edge (small $x_{\text{src}}$) (Fig. 5.12a).

Results of $F_{\Phi_G}$ suggest that at $x/h < 13$ deposition on the ground only occurs for particles released from the lower canopy region ($z_{\text{src}}/h = 1/3$; dash lines in Fig. 5.12b). For particles released at $x_{\text{src}}/h = 13.6$, $z_{\text{src}}/h = 1/3$, most deposition on the ground occurs within a short distance downstream from the source ($(x-x_{\text{src}})/h < 2$, where rapid increase is observed for blue dash line in Fig. 5.12b), whereas for particles released at $x_{\text{src}}/h \leq 9$, $z_{\text{src}}/h = 1/3$, the rate of ground deposition remains significant until $x/h \approx 13$ (red, green, and cyan dash lines in Fig. 5.12b). This behavior of $F_{\Phi_G}$ suggests that particles located in the upper canopy region ($z/h \geq 2/3$) are unlikely to penetrate down through the lower canopy and reach the ground until the positive mean vertical velocity within the canopy becomes negligible (adjustment distance of $x/h \approx 12.3$ for $\overline{w}$, see Fig. 5.2a) and the canopy-scale coherent structure containing strong sweep events has fully developed (adjustment distance of $x/h \approx 13.3$ for $z(S_{u_{\text{max}}})$, see Fig. 5.4). Specifically, for particles released at $x_{\text{src}}/h \leq 9$, $z_{\text{src}}/h \geq 2/3$, most of the airborne particles are located above the canopy at $x/h \approx 13$ (EF/AF > 0.9; red, green, and cyan dash and solid lines in Fig. 5.11b), where deposition on the ground begins to occur. Consequently, results of $F_{\Phi_G}$ collapse for these cases, and are lower than that for particles released at $x_{\text{src}}/h = 13.6$, $z_{\text{src}}/h = 1$ (red, green, and cyan dash and solid lines compared with blue dash line in Fig. 5.12b). Within the canopy region where the vertical component of TKE and the canopy-scale coherent structures have become fully developed (adjustment of $x/h \approx 10.8$ and 13.3 for $\sigma_w$ and $z(S_{u_{\text{max}}})$,
see Figs. 5.3a and 5.4), downward penetration of particles should behave similarly to that in the field interior as long as the effect of mean vertical velocity is unimportant. In other words, particles released at \( x_{\text{src}}/h > 13.3 \) should yield approximately the same \( F_{\Phi_G} \) as those released from the field interior as long as the majority of the plume close to the source \((x - x_{\text{src}})/h < 2\), where most deposition on the ground occurs\) is confined within the region where the vertical transport of particles is dominated by turbulent dispersion \( (|\vec{w}'C'|/(|\vec{w}C| + |\vec{w}'C'|) > 0.8; dark red and dark blue regions in Fig. 5.13). This requirement is satisfied for particles released at \( x_{\text{src}}/h = 13.6 \), \( z_{\text{src}}/h = 1 \) (most of the region between \( z \pm \sigma_z \) close to the source in Fig. 5.13a is in dark red and dark blue), and consequently \( F_{\Phi_G} \) for this case is similar to that for an infinite canopy \((blue and black dash lines in Fig. 5.12b). On the other hand, particles released at \( x_{\text{src}}/h = 13.6 \), \( z_{\text{src}}/h \leq 2/3 \) yield lower \( F_{\Phi_G} \) values than those released from the field interior \((blue and black solid and dash-dot lines in Fig. 5.12b), due to non-negligible contribution from mean vertical advection \( (a \text{ significant portion of the region between } z \pm \sigma_z \text{ close to the source in Fig. 5.13b, c is in colors representing } |\vec{w}'C'|/(|\vec{w}C| + |\vec{w}'C'|) < 0.6, \text{ e.g., cyan} \). The importance of mean advection with respect to turbulent transport in the vertical direction behaves consistently with the scale \( \overline{w}/\sigma_w \), as proposed in Section 5.3.

Similarly, for \( z_{\text{src}}/h = 1/3 \), particles released at \( x_{\text{src}}/h = 0 \) yield much larger \( F_{\Phi_G} \) than those released at \( x_{\text{src}}/h = 1.9 \) \((red and green dash lines in Fig. 6.10b), due to non-negligible negative mean vertical velocity \( (\overline{w}/\sigma_w < -0.1) \) at \( 0 < x/h < 1.2, z/h < 1/2 \) (Fig. 5.3b).

Recall that the escape fraction away from the source can be estimated as \( EF \approx 1 - F_{S_p} - F_{\Phi_G}. \) For particles with negligible settling velocity \( (w_s/u_* \approx 0.04 \ll 1) \), the maximum escape fraction \( (EF_{\text{max}}) \) is approximately the same as the escape fraction at the end of the domain of interest \( (x/h = 20) \), where the effect of the canopy trailing edge is negligible. Fig. 5.14 demonstrates the effects of the canopy leading edge on the maximum escape fraction \( (EF_{\text{max}}) \) as well as the fractions of particles removed by deposition on canopy elements \( (F_{S_p}) \) and the ground \( (F_{\Phi_G}) \) at \( x/h = 20 \). The model \( EF_{\text{max}} = (1 - F_{S_p} - F_{\Phi_G})_{x/h=20} \) induces uncertainties within 5\%, and thus changes in \( EF_{\text{max}} \) with respect to the case of infinite canopy can be track to changes in \( F_{S_p} \) and \( F_{\Phi_G}. \) For particles released at a given height \( (fixed \ z_{\text{src}}/h) \), \( EF_{\text{max}} \) is enhanced by moving the source location towards the leading edge \( (x_{\text{src}} \text{ decreases}) \), except for particles released at \( x_{\text{src}}/h = 0, z_{\text{src}}/h = 1/3 \) compared
with those released at \( x_{\text{src}}/h = 1.9, z_{\text{src}}/h = 1/3 \) (Fig. 5.14a). The behavior of \( \text{EF}_{\text{max}} \) suggests that infections at canopy edges are more likely to spread widely and rapidly than those in the field interior. In particular, particles released at \( x_{\text{src}}/h < 2, z_{\text{src}}/h \geq 2/3 \) yield \( \text{EF}_{\text{max}} \geq 0.94 \approx 1 \) (Fig. 5.14a), because most of the airborne particles are located above the canopy (\( \text{EF}/\text{AF} > 0.9 \)) at \( x/h \geq 6 \) (Fig. 5.11b), whereas negligible deposition on canopy and the ground occurs at \( x/h < 6 \) ("red and green dash and solid lines" in Fig. 5.12). The downstream source location \( (x_{\text{src}}/h \approx 13.6) \) required for \( F_{S_p}(x/h = 20) \) to approach the value in the case of infinite canopy is comparable with the adjustment distance of mean streamwise velocity \( (x/h \approx 13.3; \text{Fig. 5.5a}) \). The downstream source location required for \( F_{\Phi_g} \) to approach the value in the case of infinite canopy depends on the adjustment distance of \( \overline{w}/\sigma_w \) (Fig. 5.5g), which is comparable with that for \( F_{S_p} \) for particles released at the canopy top \( (z_{\text{src}}/h = 1) \), but increases for particles released at lower locations \( (z_{\text{src}}/h \text{ decreases}) \). As a result, for \( x_{\text{src}}/h = 13.6 \), particles released at \( z_{\text{src}}/h = 1 \) yield approximately the same \( \text{EF}_{\text{max}} \) as those released from the field interior, but the increase in \( \text{EF}_{\text{max}} \) with respect to that for the case of infinite canopy is enhanced as \( z_{\text{src}}/h \) decreases. These results suggest that the enhancement of \( \text{EF}_{\text{src}} \) due to release close to the canopy leading edge is particularly important for particles released in the bottom half of the canopy.

### 5.5 Conclusions

The influences of canopy leading edge on the dispersion of particles can be separated into effects on the geometry and strength of the plume away from the source. In the case of infinite canopy, the plume geometry characterized by \( \overline{z}(x - x_{\text{src}}) \) and \( \sigma_z(x - x_{\text{src}}) \) is independent of the source height \( (z_{\text{src}}/h) \) at \( (x - x_{\text{src}})/h > 8 \), whereas the plume strength is characterized by the escape fraction that depends on \( z_{\text{src}}/h \) [5]. For particles released close to the canopy leading edge \( (x_{\text{src}}/h = 0, 1.9, 9, \text{and 13.6, as investigated in this work}) \), \( \overline{z}(x - x_{\text{src}}) \) and \( \sigma_z(x - x_{\text{src}}) \) are independent of the source location \( (x_{\text{src}}, z_{\text{src}}) \) for \( x/h > 16 \). The growth rates of \( \overline{z}(x - x_{\text{src}}) \) and \( \sigma_z(x - x_{\text{src}}) \) are slower than those for the case of infinite canopy due to greater shear in the growing IBL than that above the field interior \( (\partial \overline{u}/\partial z - (\partial \overline{u}/\partial z)_{\text{inf}} > 0) \). In other words, the canopy leading edge affects the geometry of the plume away from the source through adjustment of mean flow above the canopy (i.e., the development
of IBL).

For particles released close to the canopy leading edge, the strength of the plume away from the source can also be characterized using the escape fraction. In addition to the dependence on the source height \( \frac{z_{src}}{h} \) and the importance of gravitational settling \( \frac{w_s}{u_*} \) found for particles released from the field interior [5], the escape fraction for particles released near the canopy leading edge also depends on the streamwise source location \( \frac{x_{src}}{h} \). The escape fraction is enhanced with decreasing distance from the canopy leading edge \( \frac{x_{src}}{h} \) decreases), and the effects of the canopy leading edge on the maximum escape fraction \( \text{EF}_{\text{max}} \) depends on the fraction of particles removed by deposition on canopy elements \( F_{Sp} \) and the ground \( F_{\Phi_G} \). A good model is introduced for the maximum escape fraction, \( \text{EF}_{\text{max}} \approx 1 - F_{Sp} - F_{\Phi_G} \), where \( F_{Sp} \) and \( F_{\Phi_G} \) are evaluated away from the source (e.g., at \( x/h = 20 \) for this work). The canopy leading edge affects the strength of the plume away from the source through adjustment of flow within the canopy (e.g., mean flow, TKE, and coherent structures). Changes in \( F_{Sp} \) with respect to the case of field interior is associated with strong mean streamwise velocity at the canopy leading edge. Specifically, the rebound and re-entrainment of particles parameterized in the canopy deposition model described in Appendix A are enhanced in the adjustment region where the deceleration of mean streamwise velocity within the canopy is not complete \( \frac{\partial \bar{u}}{\partial x} < 0 \). Consequently, the downstream source location required for \( F_{Sp} \) to approach the value for the case of field interior is comparable with the adjustment distance for mean streamwise velocity \( x/h = 13.3 \). Note that this conclusion suggests the importance of the canopy deposition model and thus the necessity to improve the highly empirical model described in Appendix A. Changes in \( F_{\Phi_G} \) with respect to the case of field interior is associated with positive mean vertical velocity \( \bar{w} > 0 \) within the adjustment region induced by the deceleration of mean streamwise velocity \( \frac{\partial \bar{u}}{\partial x} < 0 \). The region with non-negligible positive mean advection with respect to turbulent transport in the vertical direction is stretched more in the downstream direction for particles released in the bottom half of the canopy than in the upper half of the canopy. The downstream source location required for \( F_{\Phi_G} \) to approach the value for the case of field interior is comparable with that for \( F_{Sp} \) for particles released at the canopy top \( \frac{z_{src}}{h} = 1 \), and increases as \( \frac{z_{src}}{h} \) decreases.

The spore escape fraction is a controlling factor on the spread of plant disease
epidemics [41]. Early in a plant disease epidemic, most spores are produced and released in the bottom half of the canopy [39]. Particles released close to the canopy leading edge \( (x_{\text{src}}/h \leq 13.6) \) yield much higher maximum escape fraction \( (\text{EF}_{\text{max}}) \) than those released in the field interior. For \( x_{\text{src}}/h = 13.6 \), this effect becomes negligible for particles released at the canopy top \( (z_{\text{src}}/h) \), but is still significant for particles released inside the canopy. In particular, particles released in the bottom half of the canopy \( (x_{\text{src}}/h = 13.6, z_{\text{src}}/h = 1/3) \) yields \( \text{EF}_{\text{max}} \) about twice the value for the case of field interior. The increase of maximum escape fraction with respect to the case of field interior need to be considered for the quantification of the possibility for infections to initiate plant disease epidemics. The current design of landscape (flat ground followed by a single type of crop) represents a poor scenario, in which spores from distant locations are most likely to infect crops in the field interior (almost no deposition on canopy elements close to the canopy leading edge), demanding tremendous scouting effort. Once the field edges are infected, spores released from these infections are very likely to escape the canopy and spread across field, contributing to wide and rapid spread of plant disease. Because the same pathogenic fungal spores do not infect two different types of crops, re-arranging the landscape may optimize the scenario. For example, tall crops (e.g., maize) can be planted around short crops (e.g., soybean), so that tall crops at the field edges are less likely to be infected than those planted as large fields. In addition, the re-circulation at the trailing edge of tall crops may lead to negative mean vertical advection at the leading edge of short crops, making the majority of fungal spores deposit at field edges of the short crops. The negative mean vertical advection at the leading edge of short crops may also reduce the probability for spores released in this region to escape the canopy, suppressing the spread of diseases. For this optimized scenario, the scouting effort may be concentrated to the field edges of short crops.

In addition, the enhancement of the strength of the plume away from the source (characterized by the maximum escape fraction, \( \text{EF}_{\text{max}} \)) suggest that specifying larger mean concentration at the canopy leading edge than in the field interior may better represent an infected field. For dispersal of particles emitted from finite area sources, existing theoretical and numerical models (e.g., Chamecki and Meneveau (2011) [92], Pan et al. (2013) [12]) parameterized the source field as a constant mean concentration field at a reference height close to the canopy.
This parameterization is unrealistic within about 10 to 20 canopy heights downstream from the leading edge of a mature maize canopy, and can reach longer downstream distances for sparser canopies. The discrepancy from reality is enhanced for particles released in the bottom half of the canopy, such as pathogenic fungal spores. Comparison between canopy-resolving and canopy-modeling LES results may improve the parameterization of source field in studies of field-scale dispersion of particles.
Figure 5.2. Iso-contours of normalized mean streamwise velocity ($\bar{u}/u_*$; a), normalized streamwise gradient of mean streamwise velocity ($\partial \bar{u}/\partial x/(u_*/h)$; b), and normalized mean vertical velocity ($\bar{w}/u_*$; c) plotted in $x/h$ (downwind) and $z/h$ (vertical) space. White region indicates $|\bar{u}|/u_* < 0.1$ (a), $|\partial \bar{u}/\partial x|/(u_*/h) < 0.1$ (b), and $|\bar{w}|/u_* < 0.1$ (c), respectively. Vertical dash line in (b) indicates $x = 3L_c$, where $L_c$ is the canopy-drag length scale [8]. Canopy edge ($x/h = 0, z/h < 1$) and top ($x/h > 0, z/h = 1$) are indicated using dot lines. The region with negative mean velocity ($\bar{w} < 0$) above the canopy ($z/h >$) in (c) is due to the effect of the trailing edge.
Figure 5.3. Normalized standard deviation of vertical velocity ($\sigma_w/u_*$; a) within the canopy against normalized downstream distance from the leading edge ($x/h$) at different heights represented by lines with different symbols: $z/h = 1$ (pentagons), $5/6$ (diamonds), $2/3$ (triangles), $1/2$ (crosses), $1/3$ (circles), and $1/6$ (squares), as well as the ratio between mean and standard deviation of vertical velocity ($\bar{w}/\sigma_w$; b) plotted in $x/h$ (downwind) and $z/h$ (vertical) space. Vertical dash lines in (a) indicate $x/h = 0$ (canopy leading edge) and $x = 6L_c$, where $L_c$ is the canopy-drag length scale [8]. White region in (b) indicates $|\bar{w}|/\sigma_w < 0.1$. Canopy edge ($x/h = 0$, $z/h < 1$) and top ($x/h > 0$, $z/h = 1$) in (b) are indicated using dot lines.
Figure 5.4. The penetration depth of shear \(((1 - L_s)/h\), where \(L_s = \overline{u}_h/(\partial \overline{u}/\partial z)_h\) is the shear length scale, and subscript \(h\) indicates values at the canopy top; dash line) and the peak location of the skewness of streamwise velocity \(z(\text{Sk}_{u,\text{max}})\); solid line) against downstream distance from the leading edge \((x/h)\). Vertical dash lines indicate \(x/h = 0\) (canopy leading edge) and \(x = L_c\), where \(L_c\) is the canopy-drag length scale.
Figure 5.5. Comparison of normalized mean streamwise velocity ($\bar{u}/u_*$; $a$), normalized mean Reynolds stress ($\bar{u}'w'/u_*$; $b$), the ratio between vertical momentum fluxes transported by sweeps and ejections ($S_{4,0}/S_{2,0}$; $c$), normalized standard deviations of streamwise ($\sigma_u/u_*$; $d$), spanwise ($\sigma_v/u_*$; $e$), and vertical ($\sigma_w/u_*$; $f$) velocities, the ratio between mean and standard deviation of the vertical velocity ($\bar{w}/\sigma_w$; $g$), as well as the skewness of streamwise ($Sk_u$; $h$) and vertical ($Sk_w$; $i$) velocities against normalized height ($z/h$) at $x/h = 13.3$ (dash lines), 16 (solid lines), and 20 (dash-solid lines) with those for the case of infinite canopy (dots) [5]. Horizontal dot lines indicate the canopy top ($z/h = 1$).
Figure 5.6. Iso-contours of mean concentration integrated in crosswind direction ($\chi$) normalized by point source strength ($Q$) plotted in $x/h$ (downwind) and $z/h$ (vertical) space for particles released at $x_{src}/h = 0$, $z_{src}/h = 1$ (a), $2/3$ (b), and $1/3$ (c). Pentagram, triangle, and circle indicate point source located at $z_{src}/h = 1$, $2/3$, and $1/3$, respectively. Dots, dash lines, and plus signs indicate results for $\bar{z}/h$, $(\bar{z} \pm \sigma_{z})/h$, and the location of maximum $\chi(x, z)$ at a given $x$ ($z_{max}$), respectively.
Figure 5.7. Iso-contours of mean concentration integrated in crosswind direction ($\chi$) normalized by point source strength ($Q$) plotted in $x/h$ (downwind) and $z/h$ (vertical) space for particles released at $x_{src}/h = 1.9$, $z_{src}/h = 1$ (a), 2/3 (b), and 1/3 (c). Symbols and lines are defined in Fig. 5.6.
**Figure 5.8.** Iso-contours of mean concentration integrated in crosswind direction ($\chi$) normalized by point source strength ($Q$) plotted in $x/h$ (downwind) and $z/h$ (vertical) space for particles released at $x_{src}/h = 9$, $z_{src}/h = 1$ (a), $2/3$ (b), and $1/3$ (c). Symbols and lines are defined in Fig. 5.6.
Figure 5.9. Iso-contours of mean concentration integrated in crosswind direction ($\chi$) normalized by point source strength ($Q$) plotted in $x/h$ (downwind) and $z/h$ (vertical) space for particles released at $x_{src}/h = 13.6$, $z_{src}/h = 1$ (a), $2/3$ (b), and $1/3$ (c). Symbols and lines are defined in Fig. 5.6.
Figure 5.10. The mean height ($\bar{z}/h$; a) and depth ($\sigma_{z}/h$; b) of the plume against downstream distance from the source ($((x - x_{src})/h)$ for particles released from different locations. In addition to lines of different styles and colors defined in Fig. 5.11, black lines indicate results for the infinite canopy case [5]. Pentagram, triangle, and circle indicate point source located at $z_{src}/h = 1, 2/3$, and $1/3$, respectively.
Figure 5.11. The escape fraction (EF; $a$) and the ratio between escape and airborne fractions (EF/AF; $b$) against downstream distance from the canopy edge ($x/h$) for particles released at $z_{src}/h = 1$ (dash lines), $2/3$ (solid lines), and $1/3$ (dash-dot lines). Red, green, cyan, blue, and black lines indicate particles released from $x_{src}/h = 0, 1.99, 9, and 13.6$, respectively. Source locations ($x = x_{src}$) are marked using vertical dot lines.
Figure 5.12. The fractions of particles removed by deposition on canopy elements ($F_{Sp}$; a) and the ground ($F_{ΦG}$; b) against downstream distance from the canopy edge ($x/h$). In addition to lines of different styles and colors defined in Fig. 5.11, the black vertical dot line in (a) indicates the location $x = 3L_c$. 
Figure 5.13. Iso-contours of the importance of vertical turbulent dispersion $(\overline{w'C'}/(|wC| + |w'C'|))$ plotted in $x/h$ (downwind) and $z/h$ (vertical) space for particles released at $x_{src}/h = 13.6$, $z_{src}/h = 1$ (a), $2/3$ (b), and $1/3$ (c). Symbols and lines are defined in Fig. 5.6.
Figure 5.14. The maximum escape fraction ($\text{EF}_{\text{max}}$; a) as well as the fractions of particles removed by deposition on canopy elements ($F_{S_p}$; b) and the ground ($F_{\Phi G}$) (c) at $x/h = 20$ against normalized downstream location of the source ($x_{\text{src}}/h$). Results for particles released from the field interior ($x_{\text{src}}/h \to \infty$) are from Pan et al. (2014) [5]. Dash lines with pentagrams, solid lines with triangles, and dash-dot lines with circles indicate results for particles released at $z_{\text{src}}/h = 1$, 2/3, and 1/3, respectively.
6.1 Introduction

Dispersion of heavy particles in the atmospheric boundary layer (ABL) is an important topic in many fields of study. Transport of snow, sand, and mineral dust are of great interest in meteorology, geology, and environmental sciences [157–159]. Knowledge of dispersal of biogenic aerosols including seeds, pollens, and spores is critical for understanding plant community dynamics and for managing agricultural crops [25]. For example, seed dispersal influences plant recruitment affecting coexistence and competition in plant communities [26], while gene flow from transgenic to non-transgenic crops can occur by wind pollination [27]. Many common plant diseases are spread by pathogenic spores that disperse through the air [28]. In these and many other instances, the heavy particles of interest are released from an area source located at or near the ground surface.

Three categories of models are commonly employed to predict particle dispersion in the ABL. The first category consists of empirical models based on data from field measurements. These models are basically descriptive, addressing the shape of dispersal curves and quantitative estimations of dispersal in space [160, 161].
Extrapolating the results of these empirical models to scales larger than those used during the corresponding field measurements is sensitive to the selection of dispersal functions and estimation of parameters [162]. Empirical dispersal models generally neglect the effects of short term variations in environmental conditions such as weather and the spatial heterogeneity of landscapes. The second category consists of numerical models that describe the movements of particles in given velocity fields of air flow. Particles are either described in trajectories using a Lagrangian approach [66,67,163–166], or in spatial distributions using an Eulerian approach [81,118]. These numerical models reproduce detailed temporal and spatial evolution of particle movements under various environmental conditions. The third category consists of theoretical models based on analytical solutions to the diffusion equation of particles emitted from horizontally homogeneous sources [84–86], point or line sources [10, 87–90], and finite area sources [91,92,121]. These models assume that particles follow turbulent motions of the air except for a mean drift due to gravitational settling and that the mean flow of air parallel to the surface is horizontally homogeneous. These theoretical models provide physical insight into the particle movement process and are particularly useful in identifying the functional form of dispersal curves which determine the likelihood of long-distance transport [167].

Chamecki and Meneveau (2011) proposed an analytical solution for the dispersion of particles emitted from a finite area source for neutral conditions, considering advection, turbulent diffusion, and gravitational settling [92]. Except for gravitational settling, the problem is analogous to the solutions for evaporation from lake surfaces obtained by Sutton (1943) [168] and Frost (1946) [169]. The theory predicts particle concentration profile, plume height, and horizontal transport above a source field. Downwind from the source, the theory predicts decay in the deposition flux with distance from the source given by a power-law. The theoretical expressions, reviewed in Section 6.2.1, provide predictions that agree well with LES results of pollen dispersion [92] and measurements of spore concentrations [93].

The ABL is seldom neutral in nature. Both field measurements and numerical simulations suggest that the amount and distance of particle transport under unstable conditions in the ABL are greater than those under neutral and stable conditions [94]. In many circumstances, the release of biogenic particles such as seeds, pollens, and spores from the plant canopies into the atmosphere occurs
primarily from mid-morning through early afternoon, when the ABL is typically unstable. Including the effects of atmospheric instability in dispersion models is therefore important for many practical applications and is especially critical for predicting long-distance transport of biogenic particles. A critical question is whether the power-law behaviour of the deposition fluxes is preserved under unstable conditions. This work extends the theoretical models for neutral conditions [92] to unstable conditions, yielding expressions that combine the effects of gravitational settling and turbulence generated by shear and buoyancy on the dispersion and deposition of particles released from area sources. The proposed modifications to theoretical and numerical models are described in Sections 6.2.2 and 6.3.1 respectively. Theoretical predictions above (Section 6.3.2) and beyond (Section 6.3.3) the source field are evaluated against LES results of particle dispersion with investigation of the effects of source field size and ABL height. Predictions of ground deposition flux is also compared with those given by Godson (1958) [10] (Section 6.4.2).

6.2 Theoretical Solutions for Particle Dispersion

6.2.1 Theory for Neutral Conditions

For an area source of a finite size $L$ in the downwind direction $x$ and infinite in the crosswind direction $y$, the steady two-dimensional problem considering advection, gravitational settling, and turbulent diffusion is described by a partial differential equation for the mean concentration $\overline{C}(x,z)$,

$$\overline{\mu}(z) \frac{\partial \overline{C}}{\partial x} - w_s \frac{\partial \overline{C}}{\partial z} = \frac{\partial}{\partial z} \left( K_e(z) \frac{\partial \overline{C}}{\partial z} \right),$$

where $\overline{\mu}$ is the horizontal mean wind, $w_s$ is the particle settling velocity in the vertical direction $z$, and $K_e$ is the eddy-diffusivity. Boundary conditions are given by:

$$\overline{C}(x = 0, z) = 0,$$

$$\overline{C}(x, z \to \infty) = 0,$$

$$\overline{C}(0 < x \leq L, z = z_{0,c}) = \overline{C}_0,$$
where $C_0$ is the prescribed source concentration at the reference height $z_{0,c}$. As noted by Chamecki (2012), the lower boundary condition cannot be expected to reproduce the details of the mean concentration field at the top of the source field, and should be interpreted as a simple model intended to produce solutions in agreement with data away from the boundary (i.e. $z \gg z_{0,c}$) [121]. The problem configuration and the most important variables to be discussed below are illustrated in Fig. 6.1.

Note Eq. (6.1) is closed if the mean wind $\overline{u}(z)$ and eddy-diffusivity $K_c(z)$ profiles are specified. The following approximations are made within the atmospheric surface layer:

$$\overline{u}(z) = u_* C_p (z/z_0)^m, \quad (6.5)$$

$$K_c(z) = \frac{\kappa u_* z}{S_c}, \quad (6.6)$$

where $u_*$ is the friction velocity, $z_0$ is the roughness length, $\kappa$ is the von Kármán constant, and $S_c$ is the turbulent Schmidt number for particle concentration. For neutral conditions, Brutsaert (1982) suggested that $m = 1/7$ and $C_p = 6$ [145].

Above the source, Eq. (6.1) has a similarity solution if the parameter

$$C_1 = \frac{S_c C_p}{\kappa z_0^m} \left( \delta_{c e}^{m} \frac{d \delta_{c e}}{dx} \right) \quad (6.7)$$
is independent of $x$ and $z$, where $\delta_c(x)$ is the local plume height defined as the height at which the concentration drops to a fixed fraction of its local maximum value ($\overline{C}/\overline{C}_0 = 0.01$ is used here). Assuming $C_1$ to be constant is equivalent to assuming self-preservation of the dimensionless mean concentration profile. In essence, the mean concentration plume can be characterized by local scales $\overline{C}_0$ and $\delta_c(x)$ which are assumed to evolve slowly in space (in the present case $\overline{C}_0$ is actually constant). The turbulence time scales are much shorter, so that turbulence can always adjust to these slowly varying mean local scales. Therefore turbulence is always in equilibrium with the local scales and is dynamically similar everywhere if non-dimensionalized by these scales [170].

In this case, the analytical solution for the normalized mean concentration profile is given by:

$$g(\eta) = \frac{\overline{C}}{\overline{C}_0} = \frac{\Gamma\left(-\frac{\gamma}{m+1}, \frac{C_1}{m+1} \eta^{m+1}\right)}{\Gamma\left(-\frac{\gamma}{m+1}, \frac{C_1}{m+1} \eta_0^{m+1}\right)}, \quad (6.8)$$

where $\eta = z/\delta_c$ is the similarity variable, $\eta_0 = z_{0,c}/\delta_c$, and $\Gamma(a,x)$ is the upper incomplete gamma function [171]. The denominator in Eq. (6.8) corresponds to an integration constant enforced by the bottom boundary condition $g(\eta = \eta_0) = 1$. This constant denominator requires $\eta_0$ to be independent of $x$, or otherwise no similarity solution exists. Using a fixed $z_{0,c}$, the consequence of allowing a constant $\eta_0$ is to evaluate $\delta_c(x)$ at an appropriate location $x = x_c$ that guarantees an approximate self-preservation of $g(\eta)$. Chamecki and Meneveau (2011) used $x_c = L/2$ [92]. Here $x_c$ is interpreted as the distance from the upwind edge required for the development of the self-similar concentration profile. For dispersion from plant canopies $x_c = C_c h$, where $h$ is the canopy height, and determine $C_c$ using LES results. The scaling factor $C_c$ may depend on the characteristics of turbulence and particles. The dimensionless parameter $\gamma$ is a measure of the relative importance of gravitational settling and turbulent transport:

$$\gamma = \frac{S_c w_s}{\kappa u_*}, \quad (6.9)$$

In order to determine $C_1$, Chamecki and Meneveau (2011) modified the expression for the internal boundary layers [172] to constrain the growth rate of the
particle plume \[92]\):

\[
\frac{d\delta_c}{dx} = \frac{C_w \sigma_w(z) - w_s}{\bar{u}(z)},
\]

(6.10)

where \(C_w\) is an empirical constant that satisfies \(1.25 C_w = 0.85\) \([6]\), and \(\sigma_w(z)\) is the profile of standard deviation of vertical velocity. Both \(\sigma_w(z)\) and \(\bar{u}(z)\) are evaluated at \(z = \delta_c(x)\). Combining Eqs. (6.7) and (6.10) yields an expression for \(C_1\):

\[
C_1 = \frac{C_w \sigma_w(\delta_c) \zeta_c}{\kappa u_*} - \gamma,
\]

(6.11)

in which Chamecki and Meneveau (2011) used \(\sigma_w(z) = 1.25 u_*\) for neutral conditions \([92]\). Integration of Eq. (6.10) using the initial condition \(\delta_c(x = x_0) = 0\) yields

\[
\delta_c(x) = \left[C_1 \frac{\zeta_{z_0}^m}{\zeta_c \zeta_p} (m + 1)(x - x_0)\right]^{1/(m+1)},
\]

(6.12)

where the virtual origin \(x_0 = -64.25\) m is fitted using LES results.

Downstream of the area source, the ground deposition flux can be defined as the total vertical flux resulting from Eq. (6.1) evaluated at \(z = z_{0,c}\):

\[
\Phi(\xi) = \left[w_s \bar{C} + K_c \frac{\partial \bar{C}}{\partial z}\right]_{z = z_{0,c}},
\]

(6.13)

where \(\xi = x - L\) is the distance beyond the downwind edge of the source field. Note that this definition includes contributions due to gravitational settling and vertical turbulent diffusion, and that particle rebound and resuspension are neglected. Assuming self-preservation of the concentration profile downwind from the source (here written as \(f(\eta) = \bar{C}/\bar{C}_{max}(x)\) to emphasize that this function is different from \(g(\eta)\)), the similarity theory and the mass conservation constraint yield an expression for the ground deposition flux:

\[
\Phi(\xi) = \frac{F_T(\beta - 1)}{b \delta_L} \left[1 + \frac{1}{b} \frac{\xi}{\delta_L}\right]^{-\beta},
\]

(6.14)

where \(\delta_L\) is the plume height at \(x = L\). This expression has the same form as the modified power-law proposed by Mundt and Leonard (1985) \([173]\) that fits field measurements well \([93]\). Chamecki and Meneveau (2011) estimated the parameters
Combining Eqs. (6.14) and (6.17) suggest that for neutral conditions \( \Phi(\xi)/(u_*C_0) \) for a fixed value of \( \gamma \) only depends on \( \xi/\delta_L \) (i.e. \( \delta_L \) is the appropriate scale to characterize the effect of the source size on the deposition patterns). The fraction of particles crossing the downwind edge of the source field that remains airborne at a distance \( \xi \) is therefore given by [93]

\[
AF(\xi) = \left[ 1 + \frac{1}{b} \frac{\xi}{\delta_L} \right]^{1-\beta},
\]

which can be used to characterize dispersal distances beyond the source field.

### 6.2.2 Effects of Atmospheric Instability

Chamecki and Meneveau (2011) assumed neutral atmospheric stability in the profiles of \( \overline{w}(z) \), \( K_c(z) \), and \( \sigma_w(z) \) in their solution for the concentration profile of heavy particles above the source [92]. As the atmosphere becomes increasingly unstable, changes in \( \overline{w} \) with height become weaker, which can be accounted for by adjusting \( m \) and \( C_p \) in Eq. (6.5). Meanwhile, the standard deviation of the vertical velocity \( \sigma_w \) (and consequently the vertical diffusivity \( K_c \)) is enhanced, leading to a faster growth of the particle plume, which can be accounted for by modifying \( \sigma_w(z) \) in Eq. (6.11). Note that modifications to Eq. (6.6) would require a new solution, and are not considered in this study.
We rewrite Eq. (6.11) as

\[ C_1 = \frac{C_w \phi_w(z/L_O) S_c}{\kappa} - \gamma, \quad (6.19) \]

where \( \phi_w(z/L_O) = \sigma_w(z)/u_* \) is the dimensionless standard deviation of the vertical velocity from Monin-Obukhov similarity, and \( C_1 \) is evaluated at \( z = \delta_c(x) \) (Section 6.2.1). In the absence of water vapour, the Obukhov length \( L_O \) is defined as

\[ L_O = -\frac{u_*^3}{\kappa g a \bar{\theta}' s}, \quad (6.20) \]

where \( g_a = 9.81 \, \text{m s}^{-2} \) is the gravitational acceleration, \( \bar{\theta} \) is the mean potential temperature, and \( \bar{w}' \bar{\theta}' s \) is the surface sensible heat flux. Kaimal and Finnigan (1994) suggested that \[ \phi_w(z/L_O) = 1.25 \left( 1 + 3 \frac{z}{|L_O|} \right)^{1/3}, \quad (6.21) \]

following an equation given by Panofsky et al. (1977) [174].

For neutral conditions, as \( L_O \to -\infty \), \( \phi_w(z/L_O) = 1.25 \) and \( \sigma_w \) from Eq. (6.21) is consistent with the value used by Chamecki and Meneveau (2011) [92]. For unstable conditions, \( C_1 \) depends explicitly on \( \delta_c(x) \), violating the requirement for the assumption of self-preservation of \( g(\eta) \). An approximate constant \( C_1 \) is required to allow the theoretical solutions for \( g(\eta), \delta_c(x) \), and \( F_T \) given by Eqs. (6.8), (6.12), and (6.17) to remain applicable. Consequently, Eq. (6.19) needs to be evaluated at an appropriate \( z \), for example \( z = \delta_{c,\text{neutral}}(x = x_c) \), where \( \delta_{c,\text{neutral}} \) is given by Eq. (6.12). As the ABL becomes increasingly unstable, the enhanced growth rate of \( \delta_c(x) \) and the decreased absolute value of \( L_O \) increase the dependence of \( C_1 \) on \( x \), amplifying the departures from self-preservation. Therefore, the expectation is that the departures from self-preservation will increase with increasing atmospheric instability. Physically this can be interpreted as an increase in the turbulence time scales that can no longer adjust quickly enough to the faster evolving \( \delta_c(x) \).

In addition, \( C_1 \) increases as the atmospheric instability increases, leading to a decrease in \( g(\eta) \) at a fixed value of \( \eta \), consistent with the findings in Boehm et al. (2008) that inadequate consideration of the effects of atmospheric instability causes a significant overestimation of particle concentrations near the ground [175].
On the other hand, combining Eqs. (6.12) and (6.17) suggests that $F_T/\left(\bar{u}_sC_0\right)$ as a function of $\gamma$ is independent of $C_1$, and therefore independent of atmospheric instability.

Accepting the assumption of self-preservation of mean concentration profile for unstable conditions as an approximation of the true conditions, Eq. (6.14) can be used to predict the ground deposition flux beyond the source field. The buoyancy-generated turbulence is expected to affect deposition patterns through parameters $b$ and $\beta$. These two parameters may depend on characteristic velocity and length scales including $w_*, L_O, z_i, \delta_L, h, \text{ and } z_0$, in addition to $u_*$ and $w_*$ used in the neutral case; however, the effects of $h$ and $z_0$ are not investigated in this work. The convection velocity $w_*$ is defined as

$$w_* = \left(\frac{g_a}{\bar{\theta}} w^{*^2} \bar{\theta}^* z_i\right)^{1/3}, \quad (6.22)$$

where $z_i$ is the ABL height. Effects of atmospheric instability on $b$ and $\beta$ are investigated in Section 6.3.3.

### 6.3 Comparing Theoretical solutions with Numerical Simulations

#### 6.3.1 Description of Numerical Simulations

The three-dimensional LES model used here is described by Kumar et al. (2006) [105]. This model produces accurate velocity and temperature statistics for both neutral and unstable conditions [78,79]. Treating particles as passive scalars using an Eulerian approach, the particle dispersion results from numerical simulations under neutral conditions agree well with results from point-source and area-source release experiments [80,81]. Effects of particle inertia are neglected in the simulations on the basis of the small Stokes numbers investigated ($St = \tau_p/\tau_\eta$, where $\tau_p = w_*/g_a$ is the particle relaxation time scale and $\tau_\eta$ is the Kolmogorov time scale of the turbulence). Chamecki and Meneveau (2011) used this model to validate theoretical predictions of particle dispersion for neutral conditions [92] (the 17% increase in
settling velocity observed by Chamecki and Meneveau (2011) [92] is unrealistic\(^1\). The bottom boundary condition is prescribed by imposing a surface concentration value and using a wall layer model to determine the instantaneous vertical flux based on the resolved concentrations at the first vertical grid level. The wall model is a generalized equilibrium profile including atmospheric instability [86]. It is important to emphasize that this approach is consistent with the formulation used in the mathematical model Eq. (6.13).

Domain size and grid resolution for all simulations are listed in Table 6.1. A geostrophic wind of 8 m s\(^{-1}\) drives the velocity field. The source field used for the simulations has a finite size of \(L\) in the downwind direction and is infinite in the crosswind direction, employing a uniform height of \(h = 1\) m and a constant particle concentration of \(\overline{C}_0 = 500\) grains m\(^{-3}\) at a reference height of \(z_{0,c} = z_0 + d_0\), where \(z_0 = h/8\) is the roughness length and \(d_0 = 0.75h\) is the displacement height. The rest of the domain other than the source field is grass with a roughness length of \(z_0 = 0.01\) m. The simulation employs periodic horizontal boundary conditions except for particle concentration in the downwind direction (outflow condition).

A total of 12 simulations are conducted for four stability classes characterized by different values of surface sensible heat flux \(\overline{w'\theta'}_s\): neutral (N), weakly unstable (WU), moderately unstable (MU), and strongly unstable (SU). For the neutral (N) class \(\overline{w'\theta'}_s = 0\) K m s\(^{-1}\), and the surface sensible heat flux has increasingly positive values for the WU, MU, and SU classes, as indicated by Table 6.2. The effects of particle settling velocity are investigated for each stability class using \(w_s = 0.08\) m s\(^{-1}\) (08) for heavy particles and \(w_s = 0.02\) m s\(^{-1}\) (02) for light particles.

\(\text{Table 6.1. LES domain size and grid resolution.}\)

<table>
<thead>
<tr>
<th>Direction</th>
<th>(x) (downwind)</th>
<th>(y) (crosswind)</th>
<th>(z) (vertical)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Domain size [m]</td>
<td>3000</td>
<td>3000</td>
<td>1500</td>
</tr>
<tr>
<td>Grid points</td>
<td>150</td>
<td>150</td>
<td>500</td>
</tr>
<tr>
<td>Resolution [m]</td>
<td>20</td>
<td>20</td>
<td>3</td>
</tr>
</tbody>
</table>

\(^1\)In Chamecki and Meneveau (2011) the fluid acceleration is calculated based on the pressure gradient and the divergence of the subgrid scale (SGS) stress tensor [92]. However, the gradient of the modified pressure which includes the kinetic energy term (coming from the rotational form of the non-linear term) was used instead of the real pressure. When this term is subtracted, the effects of inertia are found to be negligible.
Assuming the Kolmogorov microscale $\eta \approx 1$ mm yields $St \approx 0.1$ for the heavier particles and the effects of particle inertia should be minor (see Chamecki and Meneveau (2011) [92] for more details). For the MU class, the effects of source size and initial ABL height are investigated for $L = 160$ m, 320 m, and 480 m in the downwind direction and initial $z_i = 855$ m and 510 m. For each case study, the velocity and temperature fields are simulated for four hours, the time it takes the turbulence to reach a statistically steady state. Then particle dispersion is simulated for 1.25 hours. The analysis of results reported here is based on the last hour of the simulation, and thus approximates steady-state conditions. The final ABL height is determined as the location of minimum sensible heat flux [79]. Parameters $m$ and $C_p$ are fitted based on Eq. (6.5) using simulated mean wind profiles in the bottom 50 m of the domain. In the analysis of simulation results, $S_c = 0.5$ is used as determined from LES results for passive scalars under neutral conditions by Chamecki and Meneveau (2011) [92].
Table 6.2. LES inputs and results of important parameters. Here $\overline{w^' \theta^'}$ is the imposed heat flux at the bottom boundary of the domain, $w_s$ is the particle settling velocity, $L$ is the size of the source field in the downwind direction, $z_i$ is the ABL height determined as the location of minimum heat flux (superscripts “initial” and “final” indicate the value prescribed at the beginning of the simulation and the value obtained during the last hour of the simulation, respectively), $L_O$ is the Obukhov length (defined by Eq. (6.20)), $u^*$ is the friction velocity, $w^*$ is the convection velocity (defined by Eq. (6.22)), $m$ and $C_p$ are used to describe the mean wind profile (Eq. (6.5)), $\gamma$ is defined by Eq. (6.9), $C_1$ is used to describe the mean concentration field above the finite area source, $\overline{C}/\overline{C}_0$ (defined by Eq. (6.27)) and $\delta_c$ (the height at which the mean concentration $\overline{C}/\overline{C}_0 = 0.01$, where $\overline{C}_0$ is the prescribed source concentration) are measures of the plume height, $b$ and $\beta$ are used to describe the mean ground deposition rate downwind from the finite area source (Eq. (6.14)), $\epsilon$ and $\beta_G$ were used by Godson (1958) [10] to describe the mean ground deposition rate downwind from a crosswind line source (Eq. (6.28)).
Simulation parameters for each case study are shown in Table 6.2. Changes in the source field size do not affect the turbulence characteristics. A lower initial \( z_i \) results in a lower final \( z_i \), affecting \( w_*, u_*, m, \) and \( C_p \). The changes in \( u_* \) then affect the values of \( L_O \) and \( \gamma \) and therefore the relative importance of turbulent transport relative to gravitational settling. Note however that the ratio \( w_*/u_* \propto (z_i/L_O)^{1/3} \) is not affected by changes in the final \( z_i \) as long as the surface heat flux is kept constant. The growth rate of the particle plume indicated by \( C_1 \) increases with increasing atmospheric instability and decreasing \( \gamma \). Discussions of parameters \( b \) and \( \beta \) are deferred to section 6.3.3 and definitions of \( z, \epsilon \) and \( \beta_G \) are deferred to section 6.4.

Fig. 6.2 shows the instantaneous and mean particle concentrations for neutral (NH08) and the strongly unstable (SUL08 and SUL02) case studies. The smooth iso-contours of mean particle concentration for all cases confirm that results are statistically well converged. As expected, the unstable atmospheric temperature stratification has profound effects on particle dispersion: the consequent large turbulent eddies increase the particle plume heights and yield more irregular instantaneous concentration iso-contours. The effect of settling velocity on the particle plume is clearly evident, even for the strongly unstable cases.

### 6.3.2 Particle Plume Above the Source

The validity of the self-preservation assumption is tested by verifying the collapse of the dimensionless particle concentration profiles at different locations. Fig. 6.3 displays the particle concentration profiles at different locations above the source for simulations NH08, NH02, WUH08, WUH02, MUH08, MUH02, SUL08, and SUL02. These selected locations are at \( x \geq 110 \) m, where the particle concentration boundary layer is fully developed. For neutral cases \((\overline{w'\theta'}_s = 0 \text{ K m s}^{-1})\), the firm validity of the self-preservation assumption implies a constant \( C_1 \), consistent with the derivation in Section 6.2.1 that summarizes the findings in Chamecki and Meneveau (2011) [92]. For unstable conditions \((\overline{w'\theta'}_s > 0)\), small departures from self-preservation are observed. These departures become more pronounced with increasing atmospheric instability, and are most noticeable in the upper part of the plume \((\eta > 1)\) where concentrations are very low, consistent with the amplified dependence of \( C_1 \) on \( x \) and the increase in turbulence time scales.
Figure 6.2. Normalized instantaneous particle concentration ($C/C_0$) iso-contours for neutral (a; NH08) and strongly unstable (c; SUL08 and e; SUL02) cases and mean particle concentration ($\overline{C}/C_0$) iso-contours for neutral (b; NH08) and strongly unstable (d; SUL08 and f; SUL02) cases plotted in $x$ (downwind) and $z$ (vertical) space. The particle source is located between the two vertical dash lines on each panel.
Figure 6.3. Dimensionless particle concentration \( g = C/C_0 \) vs normalized height \( \eta = z/\delta_c \) at different locations for LES cases NH08 and NH02 (a), WUH08 and WUH02 (b), MUH08 and MUH02 (c), and SUL08 and SUL02 (d). Black symbols indicate \( w^\prime_\theta w^\prime_s = 0 \) K m s\(^{-1}\) while grey symbols indicate \( w^\prime_\theta w^\prime_s = 0.025 \) K m s\(^{-1}\). Simulation results are displayed for locations 110 m (circles), 130 m (triangles), 170 m (squares), 210 m (diamonds), 230 m (stars), 270m (plus signs), and 310m (crosses) downwind from the leading edge of the source field.

with height discussed in Section 6.2.2. The self-preservation assumption is a good approximation for \( \eta < 1 \), even in the most unstable simulation \( (\overline{w^\prime_\theta w^\prime_s} = 0.1 \) K m s\(^{-1}\)). This approximate validity of the self-preservation assumption suggests that Eqs. (6.12) and (6.8) can be used under unstable conditions by evaluating \( C_1 \) at \( z = \delta_{c,\text{neutral}}(x = x_c) \) and \( \eta_0 \) at \( \delta_c = \delta_c(x = x_c) \).

Figs. 6.4 and 6.5 display the theoretical predictions using \( x_c = L/2 \) Chamecki and Meneveau (2011) [92] and the numerical simulation results for the particle concentration profile and plume height, respectively, above the source field for the NH08, NH02, WUH08, WUH02, MUH08, MUH02, SUL08, and SUL02 cases. The theoretical predictions are calculated using the modified \( C_1 \) value and two
sets of values for $m$ and $C_p$: those suggested by Brutsaert (1982) for neutral conditions [145] and the stability dependent values fitted from numerical simulations (Table 6.2). The effects of deviations in $m$ and $C_p$ on predictions of $g(\eta)$ and $\delta_c(x)$ are negligible, even though these deviations can affect the profile of $\overline{u}(z)$ significantly. These results are consistent with the expectation that the major effect of instability can be accounted for by modifying $\sigma_w(z)$ in Eq. (6.7). Close inspection of Fig. 6.4 reveals that for a given $w_s$, the value of $g(\eta)$ at a fixed value of $\eta$ decreases as the atmospheric instability increases, consistent with the expectation expressed in Section 6.2.2. The isolated set of circles on the far left of each panel in Fig. 6.4 represent the simulation results of $g(\eta)$ at the first vertical grid level. These results deviate from the theoretical predictions due to uncertainties in both theoretical expressions and numerical simulations. The theoretical predictions given by Eq. (6.8) are only valid for $\eta \gg \eta_0$, i.e., the regions to the right of the dash-dot lines for each simulation. In contrast, simulation results at the first grid level are unreliable due to the limited numerical resolution. Good agreement between theoretical predictions and simulation results of $g(\eta)$ is obtained for $\eta > 0.1$, where the agreement improves with increasing instability. Good agreement between theoretical predictions and simulation results of $\delta_c(x)$ is also obtained for all atmospheric stability conditions (Fig. 6.5), implying that the postulation $x_c = L/2 = 160$ m is appropriate. The plume height increases dramatically as the atmospheric instability increases, consistent with the expectation expressed in Section 6.2.2. Inspection of simulations with different field sizes (MUH08160, MUH08, and MUH08480) suggests that source size has no impact on $g(\eta)$ or $\delta_c(x)$ (not shown), implying that $x_c$ can be rewritten more appropriately as $x_c = 160h$.

As discussed in Section 6.2.1, $x_c$ can be interpreted as the distance from the upwind edge at which the flow has adjusted to the canopy and the self-preservation of particle concentration profile is first established, so that $x_c$ should depend on $h$ and be independent of $L$.

Fig. 6.6 shows the theoretical predictions and LES results for the integrated horizontal particle flux at the downwind edge of the source field. For a given source size, the theory states that $F_T/(u_\star C_0)$ as a function of $\gamma$ is universal for all neutral and unstable cases (Section 6.2.2). The theoretical predictions capture both the trend and the magnitude of LES results correctly, giving a positive relative bias less than about 15% for all cases in part due to a negative horizontal turbulent
Figure 6.4. Comparison of theoretical predictions and LES results for dimensionless particle concentration \( g = \frac{C}{C_0} \) vs normalized height \( \eta = \frac{z}{\delta_c} \) above source field for cases NH08 and NH02 (a), WUH08 and WUH02 (b), MUH08 and MUH02 (c), and SUL08 and SUL02 (d). Black circles and lines indicate \( w_s = 0 \).08 m s\(^{-1}\) while grey circles and lines indicate \( w_s = 0 \).02 m s\(^{-1}\). Circles denote numerical simulation results. Theoretical predictions using \( m = 1/7 \) and \( C_p = 6 \) are represented by solid curves while those using values of \( m \) and \( C_p \) listed in Table 6.2 are represented by dash curves. The vertical dash-dot lines denote the height at which \( \eta_0/\eta = 0 \).1.

flux at the downwind edge of the source field \( (\overline{w' C'} < 0) [176] \). The accuracy of theoretical predictions of the prefactor \( F_T/\delta_L \) in Eq. (6.14) is therefore guaranteed for the ground deposition flux \( \Phi(\xi) \) downwind.

6.3.3 Ground deposition Flux Downwind From the Source

Fig. 6.7 displays the concentration profiles at different locations downwind from the source from numerical simulations including NH08, WUH08, MUH08, and SUL08. Simulations using \( w_s = 0 \).02 m s\(^{-1}\) demonstrate the same patterns as the simulation using \( w_s = 0 \).08 m s\(^{-1}\). The self-preservation assumption of \( f(\eta) = \frac{C}{C_{max}(x)} \)
Figure 6.5. Comparison of theoretical predictions and LES results for plume height \( \delta_c \) vs downwind distance \( x \) above source field for cases NH08 and NH02 (a), WUH08 and WUH02 (b), MUH08 and MUH02 (c), and SUL08 and SUL02 (d). Black circles and lines indicate \( w_s = 0 \) \( 0.08 \text{ m s}^{-1} \) while grey circles and lines indicate \( w_s = 0.02 \text{ m s}^{-1} \). Circles denote numerical simulation results. Theoretical predictions using \( m = 1/7 \) and \( C_p = 6 \) are represented by solid curves while those using the values of \( m \) and \( C_p \) listed in Table 6.2 are represented by dash curves. The particle source is located between the two vertical dash-dot lines on each panel.

breaks down at locations where the particle plume grows beyond the atmospheric surface layer and into the mixed layer above (i.e., location \( \xi_{\text{max}} \) such that \( \delta_c(\xi = \xi_{\text{max}}) = 0.2z_i \)) as the similarity theory given by Eqs. (6.5), (6.6), and (6.21) becomes invalid. At locations where \( \delta_c < 0.2z_i \), the self-preservation assumption holds firmly for neutral conditions and approximately for unstable conditions. The deposition flux given by Eq. (6.14) is expected to be a good approximation for \( \xi < \xi_{\text{max}} \).

For the ground deposition flux \( \Phi(\xi) \), parameters \( b \) and \( \beta \) in Eq. (6.14) are determined for all numerical simulations that employ a source size of 320 m by minimizing the normalized mean-squared error between theoretical predictions and
Figure 6.6. Integrated horizontal particle fluxes at the downwind edge of the source \( (F_T/(u_\star C_0)) \) vs \( \gamma \) (a) and comparison between \( (F_T/(u_\star C_0)) \) given by Eq. (6.17) and those given by LES (b) at the downwind edge of the source. Symbols denote LES results: circles \((\circ)\) for \( \overline{w'\theta'}_s = 0 \) K m s\(^{-1}\), triangles \((\triangle)\) for \( \overline{w'\theta'}_s = 0.025 \) K m s\(^{-1}\), squares \((\square)\) for \( \overline{w'\theta'}_s = 0.05 \) K m s\(^{-1}\), and diamonds \((\diamond)\) for \( \overline{w'\theta'}_s = 0.1 \) K m s\(^{-1}\). Black symbols indicate \( w_s = 0.08 \) m s\(^{-1}\) while grey symbols indicate \( w_s = 0.02 \) m s\(^{-1}\). Open symbols denote initial \( z_i = 855 \) m while grey symbols denote initial \( z_i = 510 \) m. Symbol sizes represent source field sizes \((L)\) of 160 m \((\text{small})\), 320 m \((\text{medium})\), and 480 m \((\text{large})\). In the left panel (a), line styles represent source field sizes \((L)\) of 160 m \((\text{dash})\), 320 m \((\text{solid})\), and 480 m \((\text{dash-dot})\) for the theoretical predictions. In the right panel (b), dash line denotes a 1:1 relationship while dash-dot line represents a 15% positive relative bias.

Simulation results for \( \xi < \xi_{max} \) (Table 6.2). For a given value of surface sensible heat flux, a lower particle settling velocity leads to a greater value of \( b \) and a lower value of \( \beta \). For a fixed particle settling velocity, both \( b \) and \( \beta \) decrease as the surface sensible heat flux increases.

The effects of source size and initial ABL height on the ground deposition flux \( \Phi(\xi) \) is demonstrated in Fig. 6.8 which includes results from all numerical simulations that employ \( \overline{w'\theta'}_s = 0.05 \) K m s\(^{-1}\). The source size does not affect \( \Phi/(u_\star C_0) \) as a function of \( \xi/\delta_L \) for \( \xi < \xi_{max} \), implying that parameters \( b \) and \( \beta \) are independent of \( L \) and any other quantities derived from it (e.g., \( \delta_L \)). Based on the discussions in Section 6.2.2, the remaining parameters that may affect \( b \) and \( \beta \) include \( u_\star, w_s, w_\star, L_O, \) and \( z_i \). Dimensional analysis suggests that parameters \( b \) and \( \beta \) can only depend on two independent dimensionless groups \( w_s/u_\star \) and \( w_\star/u_\star \), whereas the other dimensionless group \( z_i/L_O \) is proportional to \((w_\star/u_\star)^3\). Parameter \( \gamma \) defined by Eq. (6.9) is proportional to \( w_s/u_\star \). For a given source size, changing the initial ABL height does not alter the ratio \( w_s/u_\star \), but \( \gamma \) changes due
Figure 6.7. Dimensionless concentration \( f = \frac{C}{C_{\text{max}}} \) vs normalized height \( \eta = \frac{z}{\delta_c} \) at different locations downwind from the source field for NH08 (a), WUH08 (b), MUH08 (c), and SUH08 (d) cases. Symbols represent distance beyond the downwind edge of the source field: 190 m (circles), 350 m (triangles), 690 m (squares), 810 m (diamonds), 1350 m (stars), 1890 m (inverted triangles), and 2570 m (asterisks). Black symbols indicate \( \xi < \xi_{\text{max}} \) while grey symbols indicate \( \xi > \xi_{\text{max}} \).

For neutral conditions, Eqs. (6.15) and (6.16) were proposed by Chamecki and Meneveau (2011) to estimate parameters \( b \) and \( \beta \) as a function of \( \gamma \) [92]. For unstable conditions, values of \( b \) and \( \beta \) listed in Table 6.2 deviate from those estimated using Eqs. (6.15) and (6.16), revealing the role of \( w_*/u_* \). The values listed in Table 6.2 suggest that the deviation of \( b \) from the neutral case is approximately a constant for each unstable case, implying that \( b \) as a function of \( \gamma \) and \( w_*/u_* \) can be written as

\[
b = 8.0 - 2.75 \gamma + b_1 \left( \frac{w_*}{u_*} \right), \tag{6.23}
\]
Figure 6.8. LES results of ground deposition flux \( \Phi/(u_\ast \overline{C}_0) \) for moderately unstable \( \left( w' \theta'_{s} = 0.05 \text{ K m s}^{-1} \right) \) vs normalized distance downwind from source field \( \xi/\delta_{L} \) using (a) initial \( z_i = 855 \) m and different values for \( L \) and (b) \( L = 320 \text{m} \) and different initial \( z_i \) values. In left panel (a), symbols denote \( L \) values and the style of the vertical lines denote where \( \xi = \xi_{\text{max}} \) for the different values of \( L \): 160 m (triangles and dash lines), 320 m (circles and solid lines), and 480 m (squares and dash-dot lines). In right panel (b), black circles and lines indicate \( w_{s} = 0.08 \text{ m s}^{-1} \) while grey circles and lines indicate \( w_{s} = 0.02 \text{ m s}^{-1} \). Open circles indicate initial \( z_i = 855 \) m, filled circles indicate initial \( z_i = 510 \) m, and the vertical lines indicate where \( \xi = \xi_{\text{max}} \) for initial \( z_i = 855 \) m (solid) and 510 m (dash).

where \( b_1(w_{s}/u_{\ast}) \) is approximately a linear function of \( w_{s}/u_{\ast} \). On the other hand, the fitted linear polynomials of \( \beta \) for all stability cases yield approximately the same value of 1.08 at \( \gamma = 0 \), implying that \( \beta \) as a function of \( \gamma \) and \( w_{s}/u_{\ast} \) can be written as

\[
\beta = 1.08 + \beta_1 \left( \frac{w_{s}}{u_{\ast}} \right) \gamma, \tag{6.24}
\]

where \( \beta_1(w_{s}/u_{\ast}) \) is approximately an exponential function of \( w_{s}/u_{\ast} \). Polynomials to estimate \( b \) and \( \beta \) are therefore fitted using the values listed in Table 6.2 based on Eqs. (6.23) and (6.24):

\[
b = 8.0 - 2.75\gamma - 1.02 \frac{w_{s}}{u_{\ast}}, \tag{6.25}
\]

\[
\beta = 1.08 + 1.25\gamma \exp \left( -0.013 \left( \frac{w_{s}}{u_{\ast}} \right)^{3} \right). \tag{6.26}
\]

Fig. 6.9 demonstrates good agreement between \( b \) and \( \beta \) given by Eqs. (6.25) and (6.26) and the values listed in Table 6.2. For neutral conditions, as \( w_{s} \to 0 \) and \( L_{O} \to -\infty \), Eqs. (6.25) and (6.26) become consistent with Eqs. (6.15) and
Figure 6.9. Comparison between parameters $b$ (a) and $\beta$ (b) given by Eqs. (6.25) and (6.26) and those listed in Table 6.2. Dash line denotes a 1:1 relationship and symbols represent different atmospheric stability conditions characterized by the value of the surface temperature flux: 0 K m s$^{-1}$ (circles), 0.025 K m s$^{-1}$ (triangles), 0.05 K m s$^{-1}$ (squares), and 0.1 K m s$^{-1}$ (diamonds). Black symbols indicate $w_s = 0.08$ m s$^{-1}$ while grey symbols indicate $w_s = 0.02$ m s$^{-1}$. Open symbols represent initial $z_i = 855$ m while filled symbols represent initial $z_i = 510$ m.

Ground deposition downwind of the source field given by the theoretical predictions and numerical simulations for NH08, NH02, WUH08, WUH02, MUH08, MUH02, SUL08, and SUL02 cases are presented in Fig. 6.10. Theoretical predictions using $b$ and $\beta$ given by Eqs. (6.25) and (6.26) agree well with those using $b$ and $\beta$ listed in Table 6.2 for $\xi < \xi_{max}$. For $\xi > \xi_{max}$, simulation results deviate from the patterns suggested by Eq. (6.14), because the similarity theory given by Eqs. (6.5), (6.6), and (6.21) becomes invalid when the particle plume grows beyond the atmospheric surface layer and extends into the mixed layer above, i.e., $\delta_c > 0.2z_i$. A second power-law regime with increasingly enlarged exponent appears with increasing atmospheric instability. The corresponding faster decay in deposition flux and increased airborne fractions imply that particles travel much farther once they reach the mixed layer. Conclusions of this observed second regime, however, should not be drawn without simulations of a much larger domain in the downwind direction (note that this second power-law is only clearly established in the most unstable case, while in the other cases the deposition flux is still transitioning to this regime at the end of the simulation domain).

The fraction of particles crossing the downwind edge of the source field that
Figure 6.10. Comparison of theoretical predictions and LES results for the ground deposition flux \( \Phi/u_\ast C_0 \) as a function of normalized distance downwind of the source field \( (\xi/\delta_L) \) for NH08 and NH02 (a), WUH08 and WUH02 (b), MUH08 and MUH02 (c), and SUL08 and SUL02 (d) cases. Circles denote numerical simulation results, solid curves represent theoretical predictions using \( b \) and \( \beta \) listed in Table 6.2, dash curves indicate theoretical predictions using \( b \) and \( \beta \) given by Eqs. (6.25) and (6.26), and the vertical dash-dot lines denote the location \( \xi = \xi_{\text{max}} \). Black circles and lines indicate \( w_s = 0.08 \) m s\(^{-1} \) while grey circles and lines indicate \( w_s = 0.02 \) m s\(^{-1} \).

remain airborne \((AF)\) is given as a function of distance in Fig. 6.11 for NH08, NH02, WUH08, WUH02, MUH08, MUH02, SUL08, and SUL02 cases. The theoretical predictions use \( b \) and \( \beta \) given by Eqs. (6.25) and (6.26). Good agreement is obtained for all stability cases when \( \xi < \xi_{\text{max}} \). The simulation results deviate from Eq. (6.18) when the particle plume grows beyond the surface layer, consistent with the patterns of deposition fluxes. An increasing number of particles remain airborne in the simulations with respect to the theoretical predictions as atmospheric instability increases.
Figure 6.11. Comparison of theoretical predictions (curves) and LES results (symbols) for the fraction of particles crossing the downwind edge of the source field that remain airborne (AF) with increasing normalized distance ($\xi/\delta_L$). Symbols (and contiguous curves) represent different atmospheric stability conditions characterized by the value of the surface sensible heat flux: 0 K m s$^{-1}$ (circles), 0.025 K m s$^{-1}$ (triangles), 0.05 K m s$^{-1}$ (squares), and 0.1 K m s$^{-1}$ (diamonds). Black symbols and solid lines indicate $w_s = 0.08$ m s$^{-1}$ while grey symbols and solid lines indicate $w_s = 0.02$ m s$^{-1}$. Left panel (a) includes NH08, NH02, WUH08, WUH02, MUH08, MUH02, SUL08, and SUL02 cases. Right panel (b) enlarges the area above the dash line in (a) for NH02, WUH02, MUH02, and SUL02 cases.

6.4 Comparison with Other Theoretical Approaches

6.4.1 Measures of Plume Height

It is common practice in the atmospheric dispersion literature [83, 177, 178] to describe the growth of the plume using the mean plume height $\overline{z}(x) = \int_{z_0}^{\infty} \overline{C} \, dz$. In the present approach, $\delta_c(x)$ is used instead. Using the local scales $\overline{C}_0$ and $\delta_c$, the definition of $\overline{z}$ can be written as

$$\overline{z}(x) = \delta_c(x) \frac{\int_{\eta_0}^{\infty} g(\eta) \eta \, d\eta}{\int_{\eta_0}^{\infty} g(\eta) \, d\eta}. \quad (6.27)$$

The self-preservation assumption implies that $g(\eta)$ and consequently the ratio $\overline{z}/\delta_c$ are both independent of $x$. Therefore, these measures of plume height are proportional to each other, and the present approach is consistent with the classical models. The constant of proportionality between the two measures of plume height $\overline{z}$ and $\delta_c$ depends on factors including settling velocity, friction velocity, and atmospheric stability, being unique for a given set of conditions. Calculation of $\delta_c$
from numerical simulations is straightforward. However, its determination from experimental data sets may be more challenging due to limited spatial sampling, experimental errors associated with small concentration measurements and the importance of concentration fluctuations at the edge of the plume. Therefore, it may be easier to first estimate \( \bar{\tau}(x) \) from experimental data and then use Eq. (6.27) to calculate \( \delta_c(x) \).

### 6.4.2 The Line-Source Solution of Rounds and Godson

In this section a comparison of deposition flux on the ground downwind from the source predicted by the present model is compared to the classical solutions for infinite line sources at a height \( H \) proposed by Rounds (1955) [87] and Godson (1958) [10] and reviewed in Pasquill and Smith (1983) [83]. A meaningful comparison is achieved by setting the line source at \( x = L \) and at a height \( H = \bar{\tau}(L) \) and focusing on the deposition far from the source (i.e., at very large \( \xi \)) where the source geometry should have negligible effect. It is interesting that Godson’s solution also predicts a deposition flux that decays as a power-law far from the source (\( \Phi_G(\xi) \sim \xi^{-\beta_G} \) for large \( \xi \)). The power-law exponent is given by

\[
\beta_G = 1 + \frac{\gamma}{\epsilon(1 + m)},
\]

where \( \epsilon \) is a correction for atmospheric stability, which can be modeled as \( \epsilon = (1 + 7 \times 0.1 \kappa (w_*/u_*)^3)^{1/3} \) [179]. Note the striking similarity between \( \beta_G \) and \( \beta \) given by Eq. (6.26), for both neutral and unstable stratification. Both exponents decrease with increasing atmospheric instability, but \( \beta \) is always slightly greater than \( \beta_G \) for a given set of conditions. A comparison between the two exponents is presented in Fig. 6.12(a) and the values of \( \beta_G \) for the simulation conditions are shown in Table 6.2. Deposition fluxes predicted by both models are compared in Fig. 6.12(b) for \( \gamma = 0.45 \) under neutral and strongly unstable conditions. Clearly the near fields are very different and reflect the different source characteristics, but the far field predictions behave similarly. The area source solutions produce large deposition at small \( \xi \), leading to faster power-law decay of deposition at large \( \xi \) compared with line sources. It is interesting to note that Godson’s model relies on the hypothesis that deposition can be modeled by a deposition velocity as suggested by Calder (1961) [180] and further assumes that this velocity is equal to the settling
velocity, which is equivalent to neglecting the second term on the right-hand side of Eq. (6.13).

### 6.5 Conclusions

This work extends the theoretical predictions of dispersion of particles emitted from a finite area source for neutral conditions proposed by Chamecki and Meneveau (2011) [92] to unstable conditions. These predictions include the mean particle concentration profiles (Eq. (6.8)), plume height (Eq. (6.12)), and horizontal transport (Eq. (6.17)) above the source and ground deposition flux (Eq. (6.14)) downwind from the source. This extension broadens the applicability of the theory proposed by Chamecki and Meneveau (2011) [92] because the atmosphere is seldom neutral. Compared with neutral conditions, particles are lifted higher and transported farther downwind under unstable conditions. In the neutral case, the friction velocity \( u_* \) and settling velocity \( w_* \) are used to characterize the dispersion patterns. The unstable atmospheric temperature stratification introduces two additional length scales, the Obukhov length \( L_O \) and the ABL height \( z_i \), where the relationship between these two scales can be expressed as a ratio between velocity scales \( u_*/w_* \), and \( w_* \) is the convection velocity. The new theoretical predictions are evaluated against LES results for four stability cases including a neutral case, a weakly unstable case, a
moderately unstable case, and a strongly unstable case. Different values of particle settling velocity, source field size, and initial ABL height are considered. The theoretical predictions agree well with LES results above the source and downwind until the particle plume begins to exceed the height of the atmospheric surface layer. At this downwind distance from the field, $\delta_c(\xi = \xi_{\text{max}}) = 0.2z_i$ and the similarity theory given by Eqs. (6.5), (6.6), and (6.21) becomes inapplicable. At locations where $\delta_c < 0.2z_i$, the self-preservation assumption of particle concentration profiles holds firmly for neutral conditions and approximately for unstable conditions, even though small departures from self-preservation are observed for unstable conditions and become more pronounced as the atmospheric instability increases, confirming that the new theoretical expressions are well applicable to the atmospheric surface layer.

Above the source, the major effects of atmospheric instability can be accounted for by adjusting the growth rate of the particle plume. Here the Obukhov length is considered in the expression of vertical velocity variance profile (Eq. (6.21)). Predictions of $g(\eta)$ and $\delta_c(x)$ are independent of source field size, but the latter is strongly affected by atmospheric instability. Downwind from the source, the effects of atmospheric instability can be accounted for by considering the ratio of velocity scales $w_*/u_*$ that measures the relative importance of buoyancy-generated turbulence and shear-generated turbulence in the expressions for parameters $b$ (Eq. (6.25)) and $\beta$ (Eq. (6.26)). The values of $b$ and $\beta$ fitted using LES results decrease with increasing instability. The power-law behaviour is shown to be very similar to the one obtained for a line-source release by Rounds (1955) [87] and Godson (1958) [10]. For $\xi > \xi_{\text{max}}$, a second steeper power-law of $\Phi(\xi)$ appears because the plume grows beyond the surface layer and extends into the mixed layer above. This effect is enhanced with increasing atmospheric instability, implying that particles disperse farther from the source. Both the theoretical model and the numerical simulations suggest that deposition curves (and consequently dispersal kernels) follow power-law behaviour under unstable atmospheric conditions, and that the effect of buoyancy produced turbulence is restricted to modifying the exponent in the power-law decay.

In this work, the area source was considered infinite in the crosswind direction, which can have an important effect of dispersion of particles in the far field ($\xi \gg L$). Chamecki (2012) proposed theoretical solutions for dispersion of particles emitted
from area sources that are finite in the crosswind direction by including the dilution of particle plume due to turbulent dispersion in the crosswind direction [121]. Similar approaches are applicable to the new solutions here.
Chapter 7  |
Conclusions

This work demonstrates the capability of LES models in reproducing measurements of turbulence statistics (up to the third order) and 3-D mean concentration field for dispersion of particles inside the plant canopy roughness sublayer (i.e., canopy-scale dispersion problem; Chapter 3). The underestimation of skewness and the stress fractions carried by strong events in earlier LES studies [53–57] has been tracked to the assumption of a constant drag coefficient in the parameterization of the canopy drag. This weakness of earlier LES models is overcome by accounting for the effect of plant reconfiguration (bending of canopy elements due to aerodynamic drag force) through a velocity-dependent drag coefficient. In addition to the reconfiguration mechanism, dependence of drag coefficient on velocity can also be induced by interference of wakes of various canopy elements (sheltering effect) [49], which may also affect the skewness of velocity fluctuations [55]. The current knowledge for the sheltering effect is very limited, based on data obtained within a small range of Reynolds number and canopy density [49]. Future laboratory and field experiments are required to understand the relative importance of the sheltering effect and the effect of reconfiguration for flexible vegetation canopies, in order to improve the model for drag coefficient.

Based on the theoretical model of 1-D linear elastic bending, a theoretical model for drag coefficient, \( C_d = \min((U/A)^B, C_{d,max}) \), was introduced in Chapter 4 for reconfiguration of flexible plants, where \( U \) is the instantaneous velocity, \( A \) is a velocity scale related to plant geometry and rigidity, and \( B \) is the Vogel number. Increasingly negative Vogel number slows the increase of drag force with increasing velocity, allowing strong events to penetration more easily into the canopy. This mechanism modifies LES results of the magnitude and position of peak skewness as
well as the stress fractions carried by strong events (large $u$). The distribution of stress fractions carried by ejections ($u' < 0$, $w' > 0$) and sweeps ($u' > 0$, $w' < 0$) also changes, because within the canopy roughness sublayer most of the strong events are sweeps. The mode of reconfiguration depends on plant geometry and rigidity, and therefore parameters $A$ and $B$ must be estimated using experimental data of turbulence statistics. The current method from Cescatti and Marcolla (2004) \cite{140} estimates $A$ and $B$ using measured profiles of mean Reynolds stress and frontal leaf area density (Appendix B), showing underestimation of the drag coefficient for flexible canopies ($B < 0$). The underestimation exceeds 50% in the bottom half of the mature maize canopy. Better methods to estimate parameters $A$ and $B$ using experimental data are required to represent the effect of reconfiguration for specific vegetation canopies of interest.

LES results suggest that the streamwise velocity skewness within the canopy is tied with the stress fractions carried by strong events. The velocity skewness, the stress fractions carried by strong events, as well as the distribution of stress fractions carried by ejections and sweeps are changeable even if first- and second-order turbulence statistics remain approximately the same (Chapters 3 and 4). These changes significantly modify the dispersion of particles within the canopy roughness sublayer (Chapter 3), suggesting strong connection among skewness, strong events associated with canopy-scale coherent structures, and dispersion. The location of peak streamwise velocity skewness ($z(\text{Sk}_{u_{\text{max}}})$) characterizes the penetration depth of canopy-scale coherent structures (Chapter 4), and can be a better characteristic length scale than the mixing length scale defined as mean velocity divided by mean shear at the canopy top. Specifically, an abrupt jump of $z(\text{Sk}_{u_{\text{max}}})$ from the ground to the canopy top is observed within about two canopy heights downstream from the canopy leading edge, coinciding with the formation of canopy-scale coherent eddies (Chapter 5). Although including non-Gaussian turbulence statistics into LSMs has not improved predictions of particle dispersion in canopy flows \cite{63,103}, the weakness of LSMs in reproducing the vertical dispersion \cite{4} may be due to inadequate representation of canopy-scale coherent structures. Further understanding of particle dispersion within the canopy roughness sublayer requires comparison of results produced by the localized near-field dispersion model \cite{62}, LSMs, and LES models. For example, theoretical solutions of mean concentration profiles can be compared with LES results to
investigate whether appropriate modifications can be made for the theoretical model to account for changes in skewness and canopy-scale coherent structures. Similar modifications can be applied to LSMs to investigate the changes in LSM results. Improved theoretical solutions and LSMs are useful for efficient estimation of the fraction of particles released from the field interior.

Theoretical frameworks for dispersion of particles on canopy (Chapters 3 and 5) and field scales (Chapter 6) have been proposed based on appropriate assumptions suggested by LES results. The plume for particles released from the field interior can be approximated using a pre-existing analytical solution if the escape fraction is known (Chapters 3). Compared with the field interior, the plume for particles released close to a canopy leading edge is different in geometry due to the development of IBL and in strength due to changes in the escape fraction (Chapter 5). Quantitative estimation of the escape fraction has been obtained using LES results for both the field interior and the canopy leading edge (Chapters 3 and 5). Results suggest larger escape fractions for particle released close to the canopy leading edge (within 13.3 canopy heights of downstream distance for particles released at the canopy top and longer downstream distance for particles released at lower locations, for the case studied in Chapter 5) than those released from the field interior. Consequently, for the dispersion of particles emitted from a finite area source, specifying larger mean concentration close to the canopy leading edge than in the field interior may better represent the source field, especially for real sources located in the bottom half of the canopy. The uncertainties induced by representing the source field as a constant mean concentration at a reference height (Chapter 6) can be investigated by comparing results produced by canopy-resolving and canopy-modeling LES approaches. This comparison may help improve the theoretical model for particle dispersion on the field scale.

Effects of the canopy leading edge on the escape fraction can be tracked to the effects on the fractions of particles removed by deposition on canopy elements and on the ground (Chapter 5). For example, the rate of deposition on canopy elements is suppressed by enhanced retention and re-entrainment of particles in the region of strong mean wind, while the rate of deposition on the ground is suppressed by non-negligible mean advection with respect to turbulent transport in the vertical direction. Despite the highly empirical canopy deposition model described in Appendix A, results suggest that significant deposition of particles on dry canopy
elements only occurs away from the edge (≥ 10 canopy heights downwind from the leading edge). This behavior suggests that scouting of infections around the edge of the field may be insufficient to monitor the development of diseases epidemics. The retention and re-entrainment of particles can be suppressed for wet canopy elements (with the presence of dew), calling for a sensitivity study with enhanced critical velocity for retention and re-entrainment. The current design of landscape (flat ground followed by a single type of crop) represents a poor scenario, in which spores from distant locations are most likely to cause infect crops in the field interior, demanding tremendous effort of scouting. In addition, spores released from infections close to the edge are very likely to escape the canopy and spread disease widely and rapidly. Re-arranging the landscape by planting tall crops (e.g., maize) around short crops (e.g., soybean) may optimize the scenario, because the same pathogenic fungal spores generally do not infect different crops. The tall crops only occupy a few canopy heights in the downwind direction, where particles are unlikely to deposit on canopy elements. At the leading edge of short crops, the mean wind has already been decelerated by the tall crops, and therefore is less likely to suppress deposition of particles. In addition, the re-circulation at the trailing edge of tall crops may lead to negative mean vertical advection at the leading edge of short crops, and therefore enhance the deposition of particles on the ground. Both effects reduce the possibility for spores to deposit on canopy elements in the field interior, which may cut the effort of disease scouting. The enhanced deposition on canopy elements and on the ground also reduces the possibility for particles released from the infections close to the leading edge of short crops to escape the canopy, suppressing the spread of disease epidemics. The optimal arrangement of landscape will be investigated by future LES studies.
Appendix A
Deposition of Particles on Canopy Elements

The rate of particle deposition on canopy elements, $S_p$, is parameterized in the LES model using a modified version of the model described by Aylor and Flesch (2001) [67]. Here, particle deposition is modeled as

$$S_p = S_{p,u} + S_{p,d} + S_{p,v},$$

(A.1)

where particles are assumed to deposit onto upward facing ($S_{p,u}$), downward facing ($S_{p,d}$), and vertical ($S_{p,v}$) surfaces of canopy elements at deposition velocities $v_{d,u}$, $v_{d,d}$, and $v_{d,v}$, respectively. For dense particles ($\rho_p \gg \rho_f$, where $\rho_p$ and $\rho_f$ are the density of particles and fluid) with diameters greater than 1 µm and negligible gravitational settling ($w_s/u_* \ll 1$), it has been shown that $v_{d,d} \ll v_{d,v} \ll v_{d,u}$ [181]. Therefore $S_{p,d}$ is neglected in view of the deposition velocity conditions described above. Deposition on the vertical surfaces is included because in the present case the mean velocity in the horizontal direction increases its importance. We further assume that the rate of deposition on upward facing surfaces $S_{p,u}$ and on vertical surfaces $S_{p,v}$ are independent from each other, with the former being dominated by gravitational settling and the latter by impaction. We then propose a canopy deposition model, which is a modified version of the model described by Aylor and Flesch (2001) [67].

The calculation of deposition rate requires information on leaf area density ($a$) and its projection coefficients ($P_x$, $P_y$, and $P_z$, described in Section 3.2.1). The rate of deposition on vertical surfaces is modeled using a rate of impaction that depends
on the instantaneous horizontal velocity,

\[ S_I = E_I (P_x + P_y) a \sqrt{\tilde{u}^2 + \tilde{v}^2} \tilde{C}. \] (A.2)

Here \( E_I \) is the impaction efficiency, which is modeled using the fit of Aylor (1982) [182] to data of impaction on a cylinder in cross flow collected by May and Clifford (1967) [183]

\[ E_I = 0.86 \left( 1 + 0.442 \text{St}^{-1.967} \right)^{-1}, \] (A.3)

where \( \text{St} \) is the Stokes number

\[ \text{St} = \left( \frac{w_s}{g} \right) \left( \sqrt{\tilde{u}^2 + \tilde{v}^2} / L_v \right). \] (A.4)

Here, \( \text{St} \) is a measure of the response of particles to the airflow around canopy elements of a characteristic length scale \( L_v \) \((L_v = 0.02 \text{ m})\), estimated by Aylor (2005) [184] and Bouvet et al. (2007) [138] as the characteristic length scale of maize stalk diameter and the projected width of the leaves, also used to estimate \( \text{Re} \) in Section 3.2.1. Airflow across a canopy element generates a boundary layer that must affect the deposition velocity. However, the lack of theoretical treatment and experimental data precludes reliable parameterization for this effect [185].

Deposition rate on horizontal surfaces \( (S_{p,u} + S_{p,d}) \) is modeled as

\[ S_{p,u} + S_{p,d} = \begin{cases} S_{p,u} = f_u P_z a w_s \tilde{C} & \text{if } \tilde{w} - w_s < 0 \\ S_{p,d} = 0 & \text{if } \tilde{w} - w_s \geq 0 \end{cases}, \] (A.5)

while the deposition rate on vertical surfaces is \( S_{p,v} = f_v S_I \). The rebound and re-entrainment of particles are modeled using retention coefficients, \( f_u \) and \( f_v \), assuming that rebound and re-entrainment of particles occur at horizontal velocities \( (\sqrt{\tilde{u}^2 + \tilde{v}^2}) \) greater than a critical value, \( V_{\text{crit}} \). Following Aylor (2005), both \( f_u \) and \( f_v \) are set to 1 if \( \sqrt{\tilde{u}^2 + \tilde{v}^2} \leq V_{\text{crit}} \) and 0 if \( \sqrt{\tilde{u}^2 + \tilde{v}^2} > V_{\text{crit}} \), where \( V_{\text{crit}} = 0.45 \text{ m s}^{-1} \) [184].

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Appendix B

Estimation of Drag Coefficient from Experimental Data

The drag coefficient \(C_d\) can be estimated by fitting experimental data to the streamwise component of the Reynolds-averaged momentum equation (ensemble average of Eq. (3.1)) for airflow through horizontally homogeneous, uniform canopies in steady state [122, 139–141]. Neglecting the horizontal component of mean pressure gradient force, the viscous term, and the Coriolis term [122, 140], the streamwise component of the ensemble average of Eq. (3.1) is reduced to

\[
\frac{\partial u' w'}{\partial z} = -a P_x C_d |u| u = -a P_x R C_d |u| u, \tag{B.1}
\]

where \(R\) is defined as \(R = \frac{C_d |u| u}{(C_d |u| u)}\) and it is a measure of the correlation between the drag coefficient and the velocity fluctuations. In order to facilitate the determination of \(C_d\) from experimental data, the assumption \(R = 1\) is usually invoked [122, 140, 141]. This assumption is good if the drag coefficient \((C_d)\) is independent of the velocity \((u)\), but may induce large uncertainties in the estimation of \(C_d\) that depends on the velocity (e.g., when reconfiguration occurs). In this Appendix, we first estimate the value of \(C_d\) using the assumption \(R = 1\), and then investigate the uncertainties of the estimation associated with the plant reconfiguration mechanism.

Using the assumption \(R = 1\), one value of \(C_d\) is obtained for each layer \((1/3 < z/h < 2/3 \text{ and } 2/3 < z/h < 1)\) and each 30-minute interval of the period 0930-1700 CDT on 10 July 2011. The values obtained are shown as circles in Fig. B.1(a). The estimated \(C_d\) show clear dependence on velocity \((|u|)\), different from the
Figure B.1. Drag coefficient \( (C_d) \) against velocity \( (|u|) \) obtained from field experimental data using the approximation \( R = 1 \) (circles) compared with models \( C_d = \text{constant} = 0.25 \) (dash line) and \( C_d = (|u|/A)^B \) \((A = 0.29 \text{ m s}^{-1}, B = -0.74; \text{solid line})\) (a) and the value of \( R \) against Vogel number \( (B) \) evaluated using experimental data measured at \( z/h = 1 \) (pentagrams), \( 2/3 \) (triangles), and \( 1/3 \) (circles) (b). In panel (b), the vertical dash line indicate the location \( B = -0.74 \).

model \( C_d = \text{constant} = 0.25 \) (dash line in Fig. B.1a). The best fit to the model \( C_d = (|u|/A)^B \) yields \( A = 0.29 \text{ m s}^{-1} \) and \( B = -0.74 \) (solid line in Fig. B.1a), although the quality of the fit is limited by the small coverage of the points in the figure.

If the model \( C_d = (|u|/A)^B \) is used to model the effect of plant reconfiguration, the value of \( R \) is given by

\[
R = \frac{|u|^{1+B}u}{|u|^B |u|^u},
\]

and it can be evaluated using experimental data for a fixed value of the Vogel number \( (B) \). Here \( R \) is quantified for the typical range of Vogel number \(-4/3 < B < 0\) for each height of measurements inside the canopy. The results are shown in Fig. B.1(b). At all heights, \( B = 0 \) implies that \( C_d \) is independent of velocity, and as expected we obtain \( R = 1 \). As \( B \) becomes more negative, the correlation between the drag coefficient and the velocity increases and the value of \( R \) becomes larger. For \( B = -0.74 \) (the value used in this work, located at the vertical line in Fig. B.1b), the mean values of \( R \) are 1.17, 1.47, and 1.99 at \( z/h = 1, 2/3, \) and \( 1/3 \), respectively. The inverse of \( R \) is an estimate of the average error in \( C_d \) due to the assumption \( R = 1 \). For example, \( C_d \) obtained for \( B = -0.74 \) at \( z/h = 1/3 \) is underestimated by approximately 50%, which is a fairly large uncertainty. These result suggest the
need to develop better methods to estimate $C_d$ from field experimental data.
Bibliography


Vita

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Ying Pan was born in Chengdu, Sichuan, China in 1982, the daughter of Zaiyi Pan and Zhen Yu. She entered Peking University at Beijing, China in 2000, and received the degree of Bachelor of Science in 2004. She entered the graduate school at Peking University in 2004, and received the degree of Master of Science in 2007. During her stay at Peking University, she worked on land-atmosphere interactions in the Department of Atmospheric Sciences. She entered the graduate school at North Carolina State University, Raleigh, North Carolina in 2007, working on atmospheric chemistry in the Department of Marine, Earth, and Atmospheric Sciences. She left North Carolina State University and entered the graduate school at the Pennsylvania State University in 2010, working on turbulence and dispersion in the Department of Meteorology. During her years at graduate schools, she has produced and contributed to the following journal publications.


